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ORIGINAL STUDY

Studies on Machine Learning-guided Prediction and Experimental Validation of Ni-doped $BaCO_3$ for Energy Applications

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Abstract

Machine learning (ML) techniques are increasingly recognized as powerful tools for accelerating the discovery of functional materials for energy applications. In this study, multiple supervised ML algorithms, including Random Forest, Support Vector Machine, Naïve Bayes, and Logistic Regression, were implemented to classify and predict oxide-based compounds with potential piezoelectric properties. Among these, the Random Forest model exhibited the best predictive performance, achieving an accuracy of 94.15 %, precision of 0.74, recall of 0.99, and a Gini coefficient of 0.93. Guided by ML predictions, $BaCO_3$ was identified as a promising candidate and further optimized through Ni doping. Experimental validation was carried out via wet-chemical synthesis, and X-ray diffraction (XRD) confirmed the formation of a polycrystalline orthorhombic phase. A clear peak shift to lower angles in Ni-doped samples confirmed successful lattice substitution, while higher Ni concentrations (15 %) induced secondary phase formation. This combined computational−experimental approach demonstrates how ML-guided screening significantly reduces cost and time, offering a scalable pathway toward the rational design of energy materials for piezoelectric and dielectric applications.

Keywords: Machine learning algorithms, Data analytics, Accuracy prediction, Crystal structure

1. Introduction

To combat the damaging effects of fossil fuels on the environment, materials for alternative energy sources are crucial. Fuel cells, photovoltaic cells, thermoelectric devices, piezoelectric devices, and others are some of the most popular green energy technologies. The most popular of these energy-generating gadgets works on the principle of piezoelectric effect. Fig. 1 represents the working of piezoelectric effect. The piezoelectric effect, which uses vibrations to convert energy from mechanical to electrical, is the fundamental idea behind piezoelectric generators.

Piezoelectric materials are crystalline substances that either deform in response to an applied voltage or generate a voltage across their ends when subjected to mechanical pressure [1]. The main advantages are room temperature preparation, easy to fabricate, used for energy generation and low cost. The electrical properties of piezoelectric materials are influenced by numerous elements, including the nature of the compound, the crystal structure, dielectric constant, mechanical quality factor, dielectric loss tangent etc. The piezoelectric effect is the basic principle underlying piezoelectric generators, which use vibrations to convert mechanical energy into electrical energy.

Conventionally, the materials are selected experimentally by using various synthesis methods [2−6], dopant material used and concentration of dopant material. Oxide-based compounds are typically chosen for piezoelectric applications because of the benefits they provide.

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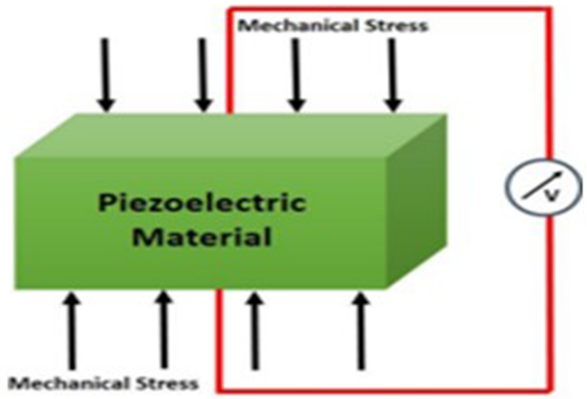

Fig. 1. Working principle of piezoelectric effect.

Lead zirconium titanate (PZT), barium titanate (BT), sodium niobate, potassium niobate, lithium niobate, and other oxide material families are said to exhibit good piezoelectric properties [7]. The demand for the creation of high-performance piezoelectric materials is rising in tandem with technological advancements. These materials must be prepared more quickly in order to satisfy increasing demands and time restrictions. Using techniques like molecular dynamics, density functional theory and Ab-initio, computational materials research helps choose the right materials. These methods contribute to the preservation of chemical resources in contrast to conventional experimental methods. However, they cost more and are time-consuming. The idea of utilizing machine learning algorithms to accelerate materials discovery is novel to materials science research community. In recent years, data analytics-based regression and classification methods have gained popularity across several fields [8−10]. They are open source, efficient, and effective. To understand the connection between a material's structure and properties, machine learning techniques will be employed. The forecast could be used to conduct experiments that have the following advantages: high predictability, reduced time, and reduced cost. Machine learning-based algorithms are used in the literature as prediction tools for solar cells, composite materials, self-healing materials, etc. [11,12]. The present work emphasizes more on implementing the potential of data analytics in materials science and also provides us a cost-effective solution for the selection of materials.

2. Methodology

The computational phase and the experimental phase are the two main stages of the process. The stages anticipated in the process during the corresponding phases are shown in Fig. 2.

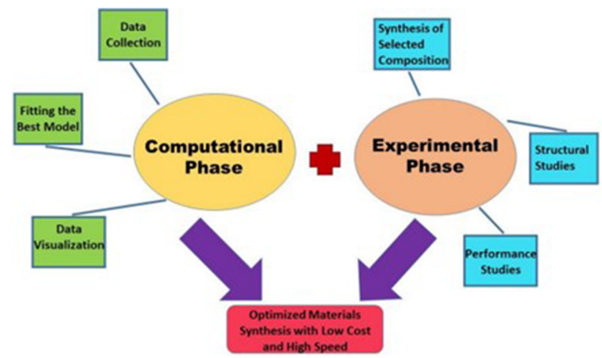

Fig. 2. Flowchart representing the phases of the project.

2.1. Computational phase

Fig. 3 represents the Plot of coefficient of determination versus types of SVM pertaining to solid oxide fuel cell materials. The corresponding coefficient of determination (R-squared or R2) along with a comparison of several SVM kernels is measured. A statistical indicator of the data's proximity to the fitted regression line is the coefficient of determination. The calculated R-squared values are almost 90 % indicating model's great accuracy in predicting new fuel cell materials.

In this phase, it is proposed to explore machine learning algorithm-based method for the screening of material families which are suitable for piezoelectric applications. Piezoelectric materials are studied for energy applications due their superior properties. The structural parameters of numerous oxide-based compounds such as the ionic radii of the cations, ionic radius of anion, the bond length, tolerance factor should be taken into consideration. To enable the model to be trained using the right machine learning

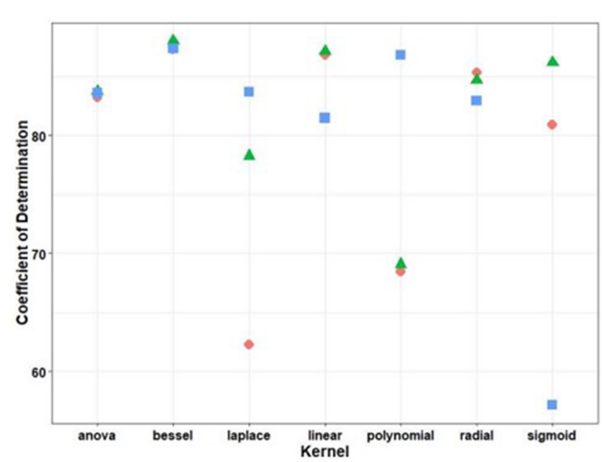

Fig. 3. Plot of coefficient of determination versus types of SVM pertaining to solid oxide fuel cell materials.

algorithms such as decision trees, Naïve Bayes Algorithm, Support vector machine and linear regression, the dataset will be separated into training and testing sets. The steps involved in classification model are Initialize the classifier, Train the classifier, Predict the target and Evaluate the model.

Naive Bayes algorithm presumes that each pair of characteristics is unique and estimates from a limited training data set. When compared to alternative techniques, it is rather quick. Baye's algorithm is stated mathematically as:

$$P(Y\,|\,Z)=\frac{P(Z|Y)}{P(Z)}$$

where Y and Z are events.

Here we are trying to find the probability of event Z, given the event Z is true. Event Z is also termed as evidence. P(Y) is the prior of Y, the prior probability, i.e., probability of event before evidence is seen. P(Y|Z) is a posteriori probability of Z, i.e., probability of event after evidence is seen.

2.1.1. Random forest algorithm

The Random Forest model uses an estimator as a parameter to estimate another model that fits many decision trees on different dataset sub-samples and uses average to get better. Data can be categorized as either structured or unstructured. Determining which group or class our data belong to is the aim of categorization.

2.1.2. Support Vector Machine

Support vector Machine (SVM) works well even with the small amount of data and gives a good result. Support vector machine helps in classification by constructing a hyperplane or set of hyperplanes. It consumes less computational power and also gives accurate results.

Table 1 shows the sample of dataset used for prediction of optimized materials for energy application. The dataset is curated from a combination of crystallographic databases (ICSD, Materials Project), and literature on oxide-based piezoelectric materials [13]. The dataset includes structural, compositional, and functional descriptors that are essential for predicting material performance. Structural descriptors such as the fractional occupancy of A- and B-site cations (A1, A2, B1, B2), ionic radii (Ra, Rb), Goldschmidt tolerance factor (TF), and lattice free volume (LFV) were derived from crystallographic data and Shannon's ionic radii database. Average bond lengths (AO) were extracted or calculated based on crystallographic information.

The methodology for data processing, model building, and performance evaluation is depicted in Fig. 4. To build the machine learning models, the response variables and feature matrices were taken out of the text data. Since the format of the raw data was consistent, we utilized the parsing technique in Java SE 14 [14]. The data was segmented into various columns and the variables was stored in arrays by developing a program with Open CSV package.

The open source programming language "R" (version 3.4.4) is utilized in this work to build the machine learning models and evaluate their performance. To properly train the models, we divided the data into 70:30 for training and testing. The data was divided using the R language's e1071 package. Popular classification methods such as Support vector machines (SVM), logistic regression (LC), Naives Bayes (NB), and random forest (RF) to build the machine learning models. SVM is a well-liked supervised classification or regression technique. The number of feature variables determines which hyper-plane in an n-dimensional plane is employed to build the SVM classifier. By choosing the hyper-plane that best divides the data classes, the classifier's performance is assessed. The kernel, C, and gamma parameters are optimized to fine-tune the SVM classifier. A method of supervised machine learning with a statistical foundation is called logistic regression. It is a popular technique for categorizing data in which the majority of the answer variable is binary. The model uses a sigmoid function to sort two or more target variables based on one or more feature variables. Naive Bayes is

Table 1. Sample of dataset used for Prediction of optimized materials for energy application.

A1	A2	Ra	B1	B2	Rb	TF	LFV	AO	RC	RELPER	D33	A1
0.95	0.05	1.5965	1	0	0.605	1.05694	4.011596	1.581593	0.814792	1030	175	0.95
0.95	0.05	1.5965	0.99	0.01	0.60615	1.056335	4.013236	1.581806	0.814975	1270	200	0.95
0.98	0.02	1.6046	0.95	0.05	0.61075	1.056767	4.024912	1.583323	0.818778	2160	210	0.98
0.95	0.05	1.5965	0.98	0.02	0.6073	1.055729	4.014876	1.582019	0.815159	1440	229	0.95
0.95	0.05	1.5965	0.97	0.03	0.60845	1.055125	4.016516	1.582233	0.815343	1580	283	0.95
0.96	0.04	1.5992	0.95	0.05	0.61075	1.054868	4.021505	1.582881	0.816735	1680	240	0.96
0.95	0.05	1.5965	0.96	0.04	0.6096	1.054521	4.018156	1.582446	0.815528	2070	338	0.95
1	0	1.61	0.9	0.1	0.6165	1.055647	4.036533	1.58483	0.821767	1680	182	1
0.95	0.05	1.5965	0.95	0.05	0.61075	1.053918	4.019797	1.582659	0.815714	1550	305	0.95
0.94	0.06	1.5938	0.95	0.05	0.61075	1.052968	4.018085	1.582437	0.814694	2650	341	0.94

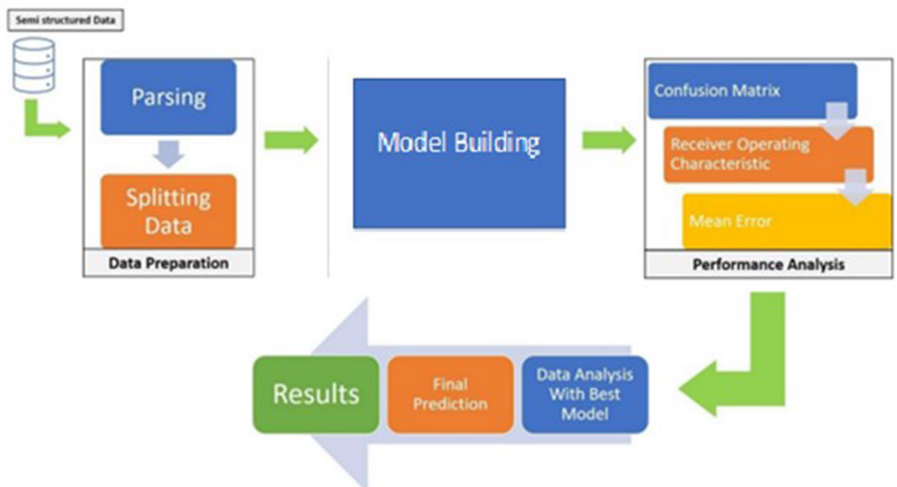

Fig. 4. Flowchart of the methodology adopted in the current study.

a successful non-linear supervised machine learning algorithm. The model utilizes the Bayes theorem for conditional probability. The random forest classification algorithm is a widely used ensemble machine learning technique due to its exceptional performance. The process creates a "forest" of decision trees, and the solution is predicted using the average outcome of each decision tree. The random forest technique minimizes over-fitting by adjusting the number of trees, number of variables randomly sampled, node size, etc. The R programming language and the e1071, caret, and random forest packages were used to build the machine learning models.

2.1.3. Evaluation of model performance

A number of evaluation standards are used to gauge the machine learning models' accuracy. For each classification model, a confusion matrix was created. The 2 × 2 matrix summarizes the true positive (TP) and true negative (TN) values along the leading diagonal. The false negative (FN) and false positive (FP) values, which stand for type I and type II mistakes, respectively, are located along the opposite diagonal. Equations (1) and (2) are used to ascertain the machine learning model's precision and recall based on the confusion matrix.

$$\text{Precision} = \text{TP}/(\text{TP}+\text{FP}) \tag{1}$$

$$\text{Recall} = \text{TP}/(\text{TP}+\text{FN}) \tag{2}$$

Equation (3) shows how the ratio of the overall quantity of values to the sum of the real positive and negative values is used to determine the model accuracy.

$$\text{Accuracy} = (\text{TP}+\text{TN})/(\text{TP}+\text{FP}+\text{TN}+\text{FN}) \tag{3}$$

The Receiver Operating Characteristics (ROC) curve is yet another essential performance indicator for assessing a classification model's quality. The curve is plotted between sensitivity and (1- specificity). Specificity, which measures the true negative rate is given by Equation (4),

$$\text{Specificity} = \text{TN}/(\text{TN}+\text{FN}) \tag{4}$$

An additional useful metric for evaluating the model's effectiveness is the area under the ROC curve (AUC). Equation (5) is employed to ascertain the Gini coefficient, which assesses the model's efficacy.

$$\text{Gini coefficient} = \mathbf{2}*\text{AUC} - \mathbf{1} \tag{5}$$

The caret and caTools packages in R programming were utilized to calculate the performance measures of the model [15–19].

2.2. Experimental phase

Chemical reagents with a stated purity of 99.99 %, such as $Ba(NO_3)_2 \cdot 3H_2O$, $Ni(NO_3)_2 \cdot 3H_2O$, NaOH, and KOH, were purchased from Merck Co. (Pharmaceutical Company, Darmstadt, Germany) and utilized without further purification. Our earlier studies describe the experimental process for creating nanomaterials with CHM.2–6 To put it briefly, a preheated furnace was used to heat a Teflon vessel holding 10 g of mixed hydroxides (NaOH:KOH = 51.5:48.5) to 200 °C. After the hydroxides were completely melted, 2.5 g of $Ba(NO_3)_2 \cdot 3H_2O$ was added, and the mixture was agitated to produce a homogenous precursor. Nickel (Ni^{2+}) doped $BaCO_3$ is effective because of the ionic radius of Ni^{2+} (0.69 Å) closely matches that of Fe^{3+}/Ba^{2+} coordination sites, enabling substitution without major

lattice distortion [20]. Ni incorporation modifies the electronic configuration and strengthens the local bonding environment, which enhances dielectric constant, reduces leakage current, and improves polarization stability.

Ni-$BaCO_3$ nanostructures (composites) with 5 % and 15 % $Ni(NO_3)_2.3H_2O$ added were also subjected to this procedure. It took over 24 h to complete. A certain amount of precursor was dissolved in varying volumes of deionized water. After aging for a few hours, the product was filtered and thoroughly cleansed with deionized water to remove any leftover hydroxides. The crystals were cleaned and then dried at 40 °C for a whole day. Based on the computational results the selected material compounds are synthesized by conventional solid state method and also wet-chemical methods such as citrate gel or Pechini method. Because they produce more homogeneity in the created compositions, which is demonstrated by superior outcomes, wet chemical techniques are preferred. Subsequent to the synthesis of the compounds, X-ray Diffraction (XRD) studies is carried out to determine the crystal structure. XRD was performed with the PANalytical diffractometer Bruker D-8 Discover X-ray diffractometer, which has a CuKα-radiation ($\lambda = 1.54186$ A).

3. Results and Discussion

The chosen supervised machine learning classification algorithms were constructed using the processed data. The process examines, contrasts, and discusses the models' performance in relation to key indicators [21]. The results are analyzed in order to determine the most suitable model which is further evaluated to predict optimized materials for energy application.

Table 2 represents the performance indicators as a function of classification model. Naive Bayes performs moderately, but has a lower AUC and Gini, meaning weaker separation of classes. Random Forest is the best model with highest accuracy, AUC, and Gini, indicating strong performance. Support Vector Machine (SVM) shows moderate accuracy, but strong AUC and Gini, meaning good classification power. Logistic Regression shows lowest performance with low AUC and Gini, making it the weakest classifier in this comparison.

Table 2. The performance indicators as a function of classification model.

Model performance	Accuracy	AUC	Gini Coefficient
Naive Bayes	77.57	0.6424	0.2848
Random forest	94.15	0.9651	0.9302
Support vector machine	77.58	0.8917	0.7834
Logistic regression	76.36	0.5450	0.0900

Fig. 5 represents the confusion matrix of various models. It is observed that the model built with random forest algorithm has an accuracy of 94.15 %. The precision and recall values of 0.74 and 0.99, respectively, further support the Random Forest model's acceptable prediction. Barium carbonate ($BaCO_3$) is the material that is most suited for energy applications, according to the RF model [22−24]. Fig. 6 represents the receiver operating characteristic (ROC) curve of various models such as Naïve Bayes, Random Forest, Support Vector Machine and Logistic Regression. ROC curves are used to evaluate the performance of classification models by plotting Sensitivity (True Positive Rate, TPR) vs. (1 - Specificity) (False Positive Rate, FPR).

Fig. 6a shows classifier that performs better than random guessing, as it deviates from the diagonal red line (which represents a random classifier). However, the curve is not very steep, indicating moderate performance. Fig. 6b belongs to a Random Forest (RF) classifier (as indicated by the legend). The curve nearly touches the upper left corner, indicating a highly accurate model with strong predictive capability. The ROC curve shown in Fig. 6c is almost a perfect diagonal, suggesting a very strong classifier with high discrimination ability. The blue line being close to the upper left suggests that the classifier is performing very well. The ROC curve (purple line) in Fig. 6d is very close to the diagonal red dashed line, indicating that this logistic regression model performs similarly to random guessing, meaning its predictive power is poor.

Fig. 7 represents the X-ray diffraction pattern of $BaCO_3$ and doped $BaCO_3$. The crystalline phases and impurity traces of the produced material are immediately tested and monitored using XRD. For both the pure and 5 % samples, every diffraction peak seen at 2θ values corresponds to the $BaCO_3$ reflection planes. The strong diffraction peaks demonstrate the formation of a single-phase polycrystalline orthorhombic BaCO3. No sample showed a diffraction peak for any impurity traces.

The $BaCO_3$ reference pattern (JCPDS# 00-005-0378) is quite similar to the obtained XRD pattern. Most of the crystallites are aligned along the (111) and (112) crystallographic planes, as seen by the peak intensities of these planes. For the 5 % nickel sample, the 2θ reflection has been shifted to a smaller angle, indicating the presence of nickel impurity at the lattice points. At the higher value of 15 % nickel content, a transition from a pure to a mixed structure was seen. The phases $BaCO_3$, $Ba(NO_3)_2$, and $Ni(NO_3)_2$ comprised the structure [25,26].

The RF algorithm provides relative importance scores for each input descriptor based on their

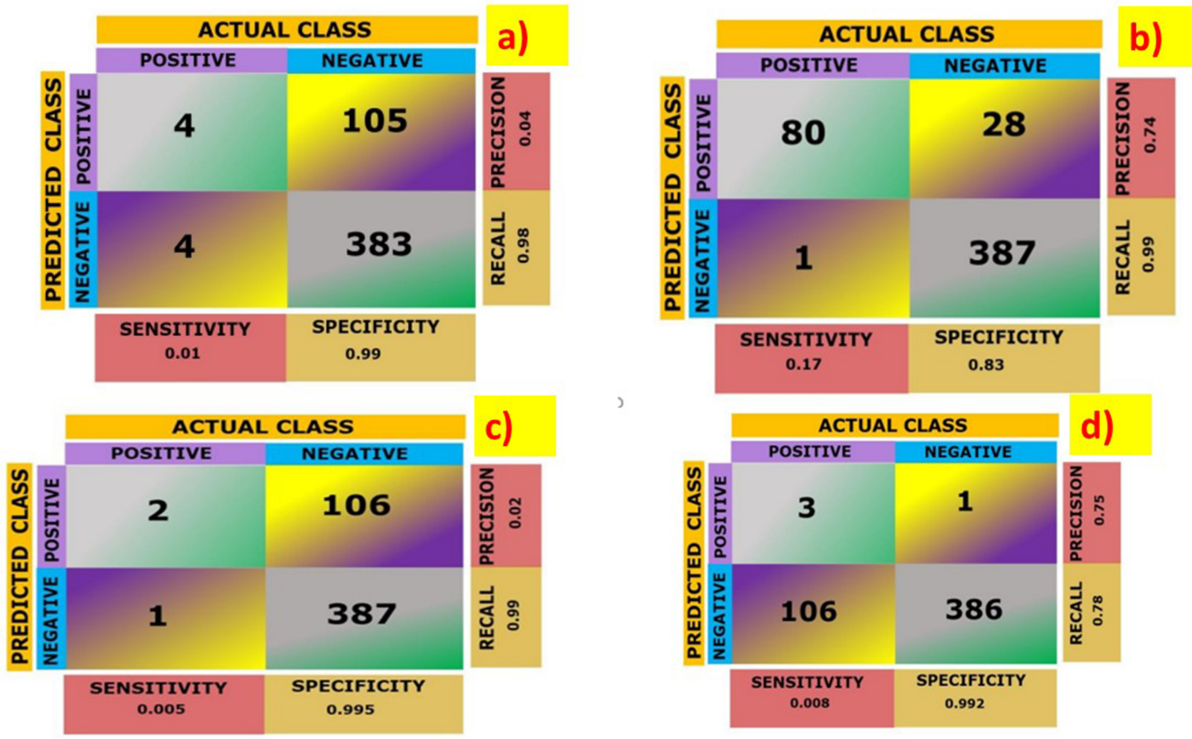

Fig. 5. Confusion matrix of various models a) Naïve Bayes b) Random Forest c) Support Vector Machine d) Logistic Regression.

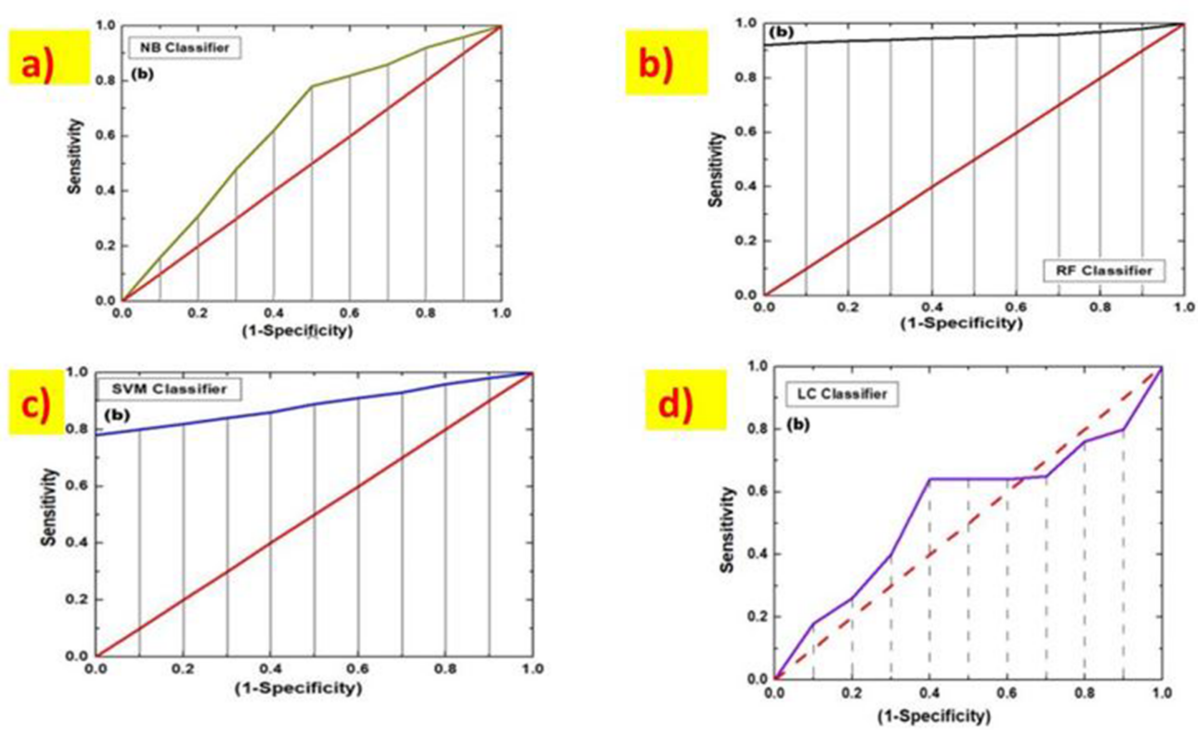

Fig. 6. Receiver Operating Characteristic (ROC) curves of various models a) Naïve Bayes b) Random Forest c) Support Vector Machine d) Logistic Regression.

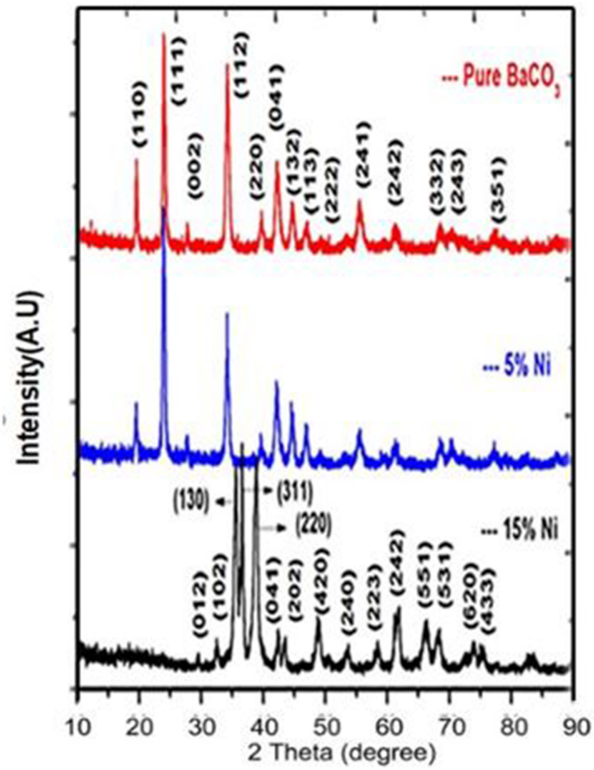

Fig. 7. X-ray diffraction pattern of $BaCO_3$ and doped $BaCO_3$.

contribution to reducing classification error. Among the considered descriptors, the tolerance factor (TF) and ionic radii (Ra, Rb) emerged as the most influential features, accounting for nearly 45 % of the model's predictive power. These features strongly influence the structural stability and distortion of perovskite-like lattices, which directly correlate with piezoelectric response. The bond length (AO) and relative permittivity (RELPER) also showed significant contributions (~30 %), reflecting their role in dielectric and polarization characteristics. Lesser importance was assigned to lattice free volume (LFV) and d_{33} coefficients, which collectively contributed ~25 %. The above analysis confirms that $BaCO_3$'s favorable tolerance factor (~1.05) and stable ionic size ratio align with the model's prediction of superior piezoelectric suitability. Moreover, the observed peak shift in XRD for Ni-doped $BaCO_3$ further supports that structural modification at the lattice level enhances the predicted performance.

3.1. Conclusion

In summary, this study demonstrates the integration of supervised machine learning (ML) algorithms with experimental validation for energy materials. Among the tested models, the Random Forest classifier achieved the highest accuracy (94.15 %) with strong precision and recall values, effectively identifying $BaCO_3$ as a promising candidate for energy-related applications. The model identified Barium Carbonate ($BaCO_3$) as a highly suitable compound for energy applications, aligning with experimental findings. XRD analysis of Ni-doped $BaCO_3$ confirmed phase formation and lattice modification, providing initial experimental support for the ML predictions. While the current validation is limited to a single material system, the findings highlight the potential of ML-guided approaches to accelerate material screening and reduce cost and time compared to conventional methods. Future work will expand this framework to additional material families and dopant levels to further establish the robustness and generalizability of ML-based material discovery.

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Conflict of interest

None.

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