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ABSTRACT

Lattice constant mismatch between materials affects the quality of thin film fabrication. For this reason, lattice constants information is vital in the design of materials for technological applications. The determination of lattice constants via experimental analysis is relatively expensive and laborious. As a result, several linear empirical models have been proposed to predict the lattice constant of crystal structures. However, the accuracies of these models are limited partly due to their failure to account for nonlinearity in the atomic parameters-lattice constant relationship. Machine learning techniques have shown excellent ability to deal with nonlinear problems in many areas of materials science; hence, they are considered suitable computation tools to study the crystal structure of materials. In this contribution, we developed a support vector regression (SVR) model to predict the lattice constant of cubic crystals of the form A_2XY_6 (A = K, Cs, Rb, TI; X = tetravalent cation; and Y = F, Cl, Br, I). The SVR algorithm uses the ionic radii and electronegativities data of the constituent elements of A_2XY_6 cubic crystals as model inputs. The robustness of the proposed model was demonstrated by comparing our result with an existing linear model based on 26 cubic crystal samples. The result revealed a total relative deviation of 1.757 and 2.704 for the SVR model and the existing linear equation, respectively. This result proves that the SVR model has a huge potential in the search for new materials for different applications.

I. INTRODUCTION

The lattice constant is an integral unit cell parameter of any crystalline substance. It can, in conjunction with other associated parameters like the site occupancy of adjoining atoms and atomic positions, give a complete description of the crystalline structure. The importance of a lattice constant is enormous, especially in material identification and structural characterization.[1] Minimizing the lattice mismatch enhances[2] the production of top-quality thin films,[3] while an increased lattice mismatch between materials can lead to an increase in the concentration of residual carriers as well as reduction of the quality of the crystal.[4]

The lattice constant depends on different variables such as ionic radii, electronegativity, and oxidation states, which are a function of the inter-ionic distance. The strong linkage between the inter-ionic distance and lattice constant is the reason why the three variables can be used to estimate the value of the lattice constant. While the ionic radii relate to the influence of geometry on the inter-ionic separation of the compound, the electronegativity considers the nature of the atomic bonding, thereby giving the model an additional detail required to provide a complete picture of the functional value of the lattice constant. An illustration of this can be seen in Cs_2GeF_6 and Cs_2MnF_6, where Ge^{4+} and $Mn4^+$ possess

the same ionic radii but have different lattice constants. The difference in their lattice constant is established to be the difference in their electronegativity.[5]

Structural determination of crystalline materials has been achieved through experimentation and theoretical investigation. X-ray crystallographic analysis and patterns from neutron diffraction findings provide robust information on crystalline structures as reliable experimental techniques, while *ab initio* computational calculations provide the theoretical framework an alternative source of crystallographic data. Currently, there is an enormous pool of veritable structural information on crystalline materials derivable through experimental findings and theoretical computations with insignificance difference often about 1%. Despite the success of crystalline structural determination, the ability to obtain fast, real-time values of lattice constants with enhanced accurate data is a major concern. Also, it is important to be able to project structural parameters of new crystals without having to restart a new experimental procedure and theoretical investigation. This line of thought cannot be wished away when we consider the cost, complexity, and time consumed by existing procedures. Experimental determination using the X-ray diffraction technique[6] can be very complex. Also, chemical stoichiometry based prediction tools (e.g., SPuDS)[7] and density functional theory-based computational tools[8–11] have been successful, but their need for high computational resources[12] is a major concern.

Recently, simple mathematical models that explore the relationship between a lattice parameter and the underlying chemical information of constituent elements have been developed.[5,13] Some of the chemical information include electronegativity, ionic radii, oxidation state, etc. They are readily available and obtainable. The beauty of these empirical models is their ability to predict lattice constants for materials that have not been previously determined experimentally. This will enable materials scientists to make informed choices on appropriate substrates that can be employed for the growth of thin films. Some successful efforts have been geared toward the use of an empirical model in estimating the lattice constant of crystalline structures. Empirical modeling of various cubic perovskite where the relationship between lattice constants and other variables such as valence electron number, ionic radii, etc., has been established.[14–18] Also, the functional relationship between lattice constants of secondary and ternary spinel compounds with electronegativity and ionic radii have also been carried out.[5]

Apart from experimental and quantum methods, the use of empirical models[14,19,20] that are based on multiple linear regression has also gained tremendous interest. These models employ linear regression techniquess[16,20] for lattice constant prediction. However, these do not account for any inherent nonlinearity in the correlation of the atomic parameters to the lattice constant, thereby not giving the complete accurate picture of the relationship. This setback necessitates the introduction of a computational intelligence (CI) approach that can handle the nonlinear patterns among the input-output data thereby increasing the accuracy of the lattice constant prediction.

Machine learning techniques have tremendously improved the characterization of materials using basic physiochemical information as descriptors. These descriptors aid the prediction of the structural features of the material. To overcome the challenges faced by existing methods, computational intelligence based methodologies such as an artificial neural network (ANN), a generalized regression neural network (GRNN), and support vector regression (SVR) have been applied in the modeling and prediction of lattice constants.[21] They are better when it comes to the prediction of the structure of novel compounds, especially in an environment of low computational resources. Among these CI-based approaches, SVR has unique merits as a result of its high generalization capability[22] and low temporal cost.[23]

The relevance of a lattice constant to the structural properties of crystals has been examined for different forms of cubic structures, such as perovskites[7,15,18,24] and the spinel compounds.[5] They are of the form A_2XY_6 (A represents K, Cs, TI, Rb; X represents the tetravalent cation; and Y represents halogens F, Cl, Br, I). This structural group is an important cubic crystal of choice, because of the easiness with which it dopes with impurity ions. They belong to the Fm-3m space group with each of its unit cells containing four formula units. Looking at its coordinate geometry, the cation A is positioned at (0.25, 0.25, 0.25), the X cation is located at the origin (0, 0, 0), and the halogen ion Y occupies (y, 0, 0), with y being different for each structure. In evaluating the parameters that characterize the lattice constant, a critical look at the geometry and nature of the inter-ionic interaction is necessary. In this cubic crystal, the p states of the halogen ion form the valence band, while the s states of the cation form the conduction band. With this arrangement, the Columbic interaction is a major precursor for the kind of bonding in the structure. It can be easily deduced that ionic radii and electronegativity will be the major descriptors for the lattice constant prediction. In this contribution, we applied SVR to predict the lattice constant of A_2XY_6 cubic crystals and compare our results with experimental and empirical results.[13]

II. MATERIALS AND METHODS

The statistical details of the data used for the modeling are presented in Table I. The data were obtained from Ref. 13. Altogether, the total number of samples used for the model development consists of 85 datasets. In terms of the anion composition, the dataset consists of 41 chlorides, 18 bromides, 17 fluorides, and 9 iodines. The model inputs comprise of the ionic radii and electronegativities of the constituent elements, while the output is the lattice constant of a series of A_2XY_6 cubic crystals. It is crucial that the model inputs chosen should have a physical relationship with the desired output. As mentioned earlier, it is well reported that the ionic radius of a compound has a strong relationship with the lattice constant.[12] However, only the ionic radii do not give a full account of the lattice constant.[13] Hence, the electronegativity information of these elements also contributes to the values of the lattice constant. Therefore, both parameters were used as inputs in this study. Table II provides the Pearson correlation between the inputs and the lattice constant. An examination of the data revealed that the ionic radii have a significant correlation coefficient with the lattice constant, which thus suggests that the ionic radii will have a major impact as a model descriptor. On the contrary, the electronegativities exhibit a relatively weaker correlation coefficient than the ionic radii, with the exception of the anion electronegativities that have a strong correlation with the lattice constant.

TABLE I. Basic statistical description of the dataset for cubic crystals of the form A_2XY_6.

Parameters	Parameters type	No of samples	Mean	Min	Max	Range
Input	R_A (Å)	85	1.7581	1.64	1.88	0.24
	R_X (Å)	85	0.6591	0.4	0.97	0.57
	R_Y (Å)	85	1.7871	1.33	2.2	0.87
	χ_A	85	0.8779	0.79	1.8	1.01
	χ_X	85	1.9296	1.30	2.55	1.25
	χ_Y	85	3.2287	2.66	3.98	1.32
Target (lattice constant)	A	85	10.037	8.109	11.790	3.681

A. Methodology

1. Support vector regression (SVR)

Support vector machine (SVM) is a machine learning technique founded on the idea of a statistical learning theory utilizing the structural risk principles. The original underlying principle of SVR was credited to Vapnik and his co-workers at the AT&T Bell Laboratories.[25] SVM has unique features that enhance its applications. These include the ability to converge to global minimum, effective learning in sparse, high-dimensional space with a small training dataset, and, more importantly, good generalization ability on a new dataset.[26,27]

Initially, the SVM was formulated to handle classification problems but later modified to solve the regression task through the use of an epsilon-insensitive loss function; in this sense, it is referred to as the ϵ-support vector regression (ϵ-SVR). Suppose we have a training dataset defined as $\{(x_1, y_1), \ldots, (x_l, y_l)\} \subset \chi \times R^d$. The main objective of ϵ-SVR is to find a function $f(x)$ that computes the dependency relationship between the input features and the target as expressed in Eq. (1),

$$y = f(x) = w \cdot x + b, \tag{1}$$

where w is referred to as weight vector, x as the input vectors, and b is the bias. The function $f(x)$ is assumed to have at most a deviation of ϵ from the actual targets y_i for all training data. In addition, such a function is expected to be as flat as possible.[28] The flatness of the function means that we seek a small w, which is done by minimizing the norm w^2.

TABLE II. Pearson's correlation coefficients (r) and p-values between the model inputs and lattice constants.

Relationships between input and output parameters	r^2	p
Lattice constant and R_A	0.341	0.001
Lattice constant and R_X	0.636	0.000
Lattice constant and R_Y	0.951	0.000
Lattice constant and χ_A	−0.127	0.247
Lattice constant and χ_X	0.094	0.393
Lattice constant and χ_Y	−0.939	0.000

This can be written as a convex optimization problem as shown below,

$$\text{minimize} \quad \frac{1}{2}\,||w||^2, \tag{2}$$

$$\text{subject to} \begin{cases} y_i - \langle w, x_i\rangle - b \le \epsilon, \\ \langle w, x_i\rangle + b - y_i \le \epsilon. \end{cases}$$

The constraint indicates that the difference between the prediction and the actual values should be less than or equal to ϵ. But, in general, due to the presence of outliers in the dataset, the deviation may be higher than ϵ; hence, the slack variables ξ_i and ξ_i^* are introduced to accommodate this constraint.[29–31] The equation can be restated as shown in (3),

$$\text{minimize} \quad \frac{1}{2}\,||w||^2 + C\sum_{i=1}^{n}(\xi_i + \xi_i^*), \tag{3}$$

$$\text{subject to} \begin{cases} y_i - \langle w, x_i\rangle - b \le \epsilon + \xi_i, \\ \langle w, x_i\rangle + b - y_i \le \epsilon + \xi_i^*, \\ \xi_i\ \xi_i^* \ge 0 \quad i = 1, 2, \ldots, n, \end{cases}$$

where C refers to the box constraint or the penalty term imposed on the objective function as a result of the introduction of the slacked variables.

The $\frac{1}{2}\,||w||^2$ represents the regularization factor, while the slack variables ξ_i and ξ_i^* represent the lower and upper bound of the excess deviations.[32] The choice of C is important because it controls the trade-off between the error tolerance (ϵ) and the model complexity. A simple function may fail to truly capture the complexity of the task, thus giving poor model predictions, while a function that gives a very little error for the training dataset may have overfitted the training data, consequently failing to give good prediction results on a new dataset.[26]

The above constraint is solved by constructing a Langrangin function from (3). For conciseness, we have have not included the details here, but interested readers can refer to Ref. 32,

$$\text{In the final analysis,}\ w = \sum_i^n (\propto_i - \propto_i^*)x_i, \tag{4}$$

where $\propto_i$ and $\propto_i^*$ refer to the Lagrange multipliers. Equation (4) refers to the support vector expansion, which implies that

w can be fully described as a linear combination of the training patterns x.

It follows that

$$f(x) = \sum_i^n (\propto_i - \propto_i^*)\langle x_i , x\rangle + b. \quad (5)$$

Equation (5) revealed that the algorithm can be fully expressed in terms of dot products between the data. For nonlinear training data, the input data are first transformed into a higher dimensional space using the kernel function. For nonlinear training data,

$$f(x) = \sum_i^n (\propto_i - \propto_i^*)\langle \varphi(x_i), \varphi(x)\rangle + b, \quad (6)$$

where $\varphi(x_i)$ and $\varphi(x)$ can be expressed in the form of a kernel function,

$$\langle \varphi(x_i), \varphi(x)\rangle = k(x_i\, x).$$

Examples of a commonly used kernel function are stated below:

- Gaussian or radial basis function (RBF): $K(x_i,\ x_j) = \exp(-\gamma.|x_i, x_j|^2)$;
- Linear: $K(x_i,\ x_j) = K(x_i,\ x_j)$;
- Polynomial: $K(x_i\ ,\ x_j) = [(x_i\ ,\ x_j) + 1]^d\ \gamma\ >\ 0$.

where γ refers to the kernel parameter.

2. Bayesian optimization

The following SVR hyperparameters affect the prediction accuracy of the SVR model performance; box constraint, the epsilon (ϵ), and the kernel function. Their values have been traditionally selected using a trial and error approach, which is not only time consuming but also less accurate.[33] These challenges are resolved using optimization techniques that are able to automatically make a selection of the best SVR hyperparameter values for a given problem. Common examples of the techniques employed include Particle Swarm Optimization (PSO),[34] Genetic Algorithm (GA),[35] Firefly Algorithm (FAA),[36] Artificial Bee Colony (ABC),[37] etc. All these techniques improve the accuracy of the machine learning algorithms as well as eradicate the laborious exercise of manually tuning the hyperparameters.

In this study, we utilized a less common but very powerful technique known as the Bayesian optimization algorithm found in the MATLAB toolbox for the selection of the optimum SVR hyperparameters values that minimize the cross-validation loss on the training dataset. Bayesian optimization makes use of an internally maintained Gaussian process model to describe the objective function, which we seek to minimize. It uses the evaluation of the objective function to train the SVR models. This evaluation process is controlled by an acquisition function that determines the next point of evaluation by making a smart decision between exploration (searching area with high uncertainty) and exploitation (the searching region with high certainty). The unique advantage of Bayesian optimization is that it makes use of the information derived from the previous evaluation of the objective function to determine the next point of evaluation, thus making it very efficient and consequently able to save significant computational power. Further details on the optimization process can be found in the literature.[38–42]

TABLE III. Bayesian optimization parameters.

Bayesian optimization settings	Values
Acqusition function name	expected improvement plus
Number of objective evaluations	100
Exploration ratio	0.5
Optimization function	bayesopt
Numseedpoints	4

3. Computational procedure

The computational work in this study was carried out in the MATLAB 2019a platform. The SVR hyperparameters were optimized using the Bayesian optimization function with parameter settings as stated in Table III. The acquired data were randomized and divided into two sections in the ratio 70:30 for the training and testing datasets, respectively. The training data were used for learning the relationship between inputs and the lattice constant. In order to reduce the risk of overfitting, we applied the 5-fold cross-validation technique during the training phase. While training the model, the optimization function evaluates various values of the box constraint, epsilon, and kernel parameters with the aim of selecting the set of hyperparameters with the least cross-validation error on the training dataset. One hundred (100) evaluations of the objective function were performed, and the optimum SVR hyperparameters obtained are presented in Table IV. The obtained optimum SVR hyperparameters were then used to make lattice constant predictions on the testing dataset.

III. RESULTS AND DISCUSSION

The lattice constant is a function of ionic radii and electronegativity values of the constituent elements, but the exact functional form of the relationships between the lattice constant and these variables is unknown. Previous studies have developed linear correlations between lattice constants and the crystal structure parameters such as ionic radii, valence, and electronegativity parameters of the constituent elements. In addition, neural network models have also been used with the crystal structure parameters for the prediction of lattice constants.[43]

In this study, we systematically investigate how each of the ionic radii and the electronegativities of the crystal elements affects

TABLE IV. Optimum SVR hyperparameters for prediction of the lattice constant of cubic crystals.

SVR hyperparameters	Values
Box constraint	53.483
Epsilon	0.0290
Kernel function	gaussian
Kernel scale	1.888

TABLE V. Results of using various input combinations for prediction of the lattice constant of A_2XY_6 crystals.

S/N	R_A	R_X	R_Y	χ_A	χ_X	χ_Y	AARD	R^2
Model 1	✓	✓	✓	x	x	x	0.9953	98.74
Model II	x	X	x	✓	✓	✓	2.0485	97.22
Model III	✓	✓	✓	✓	✓	✓	0.8225	99.07
Model IV	✓	✓	✓	✓	✓	x	0.7017	99.57

the prediction accuracy of the lattice constant of cubic crystals of the form A_2XY_6. Table V shows the summarized results of using different input combinations to model the lattice constant of the considered crystal structures. As observed, using only electronegativities of the constituents (model II) is clearly not sufficient to model the lattice constant values because it gives the highest average absolute relative deviation (AARD). Using only the ionic radii (model I) clearly shows a major improvement in terms of the prediction accuracy. This means that ionic radii of constituent elements of A_2XY_6 crystals carry significant information about the lattice constant. Both these observations are consistent with the statistical analysis conducted in Table II, where the ionic radii of the crystal structures exhibit a very high correlation coefficient while the electronegativities show a weaker correlation with the lattice constant. As expected, a combination of both ionic radii and electronegativities of the crystals' constituent elements provides a much better account of the lattice constant of the considered crystals. More importantly, the highest prediction results were obtained by excluding the electronegativity information (χ_Y) of the anion as one of the model inputs (model IV). This implies that for A_2XY_6 crystals, the most effective parameters to predict the lattice constants are R_A, R_X, R_Y, χ_A, and χ_X. Although there is a strong correlation coefficient of −0.939 between the anions and the lattice constant, yet the SVR algorithm excludes this feature as part of its input in model IV. This observation is not surprising because the parameter (χ_Y) has the same values for all the members of group VII elements. Hence, it is essentially a redundant variable that adds no benefit to the model performance. We observed a tangible improvement in the prediction accuracy when the electronegativities of the anions are excluded as a model input.

Since model IV yielded the best prediction of the lattice constant of A_2XY_6 cubic crystals, the rest of this section discusses the results obtained from model IV. Figures 1 and 2 show the cross-plots between the predicted and experimental values of lattice constants for the training and testing datasets, respectively. The results showed very high correlation rates of 99.87% and 99.57% during the training and testing phase, respectively. The degree of agreement between the experimental and predicted values is illustrated in Fig. 3 for the training dataset. Virtually, all the predicted results

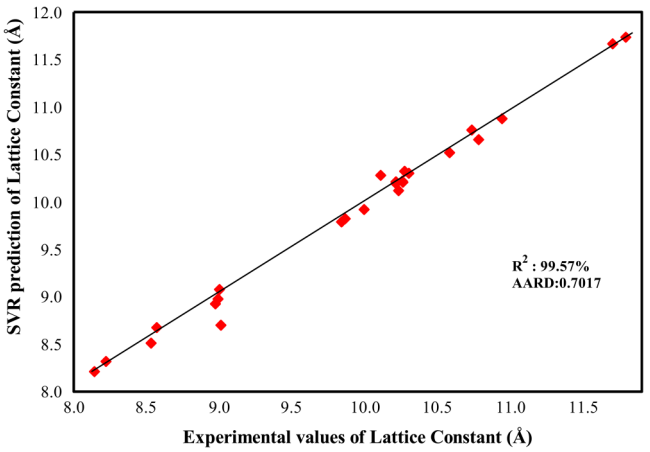

FIG. 2. Cross-plot between SVR prediction of lattice constants and the experimental values of lattice constants (testing dataset).

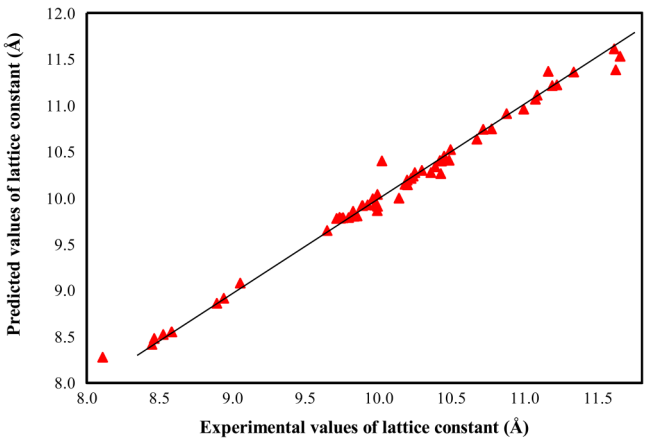

FIG. 1. Cross-plot between SVR prediction of lattice constants and the experimental values of lattice constants (training dataset).

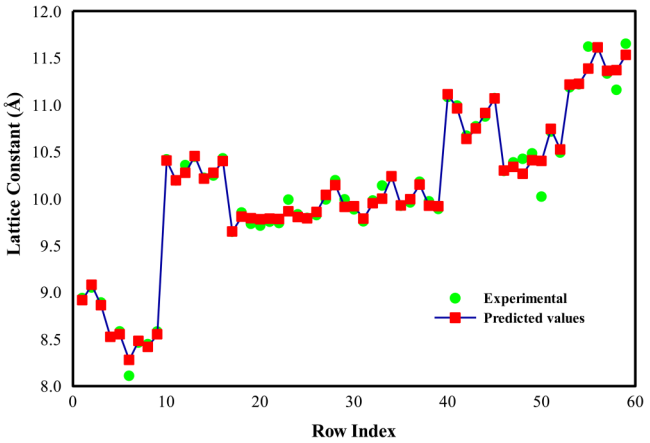

FIG. 3. Relationship between predicted and experimental values of lattice constants of the training dataset.

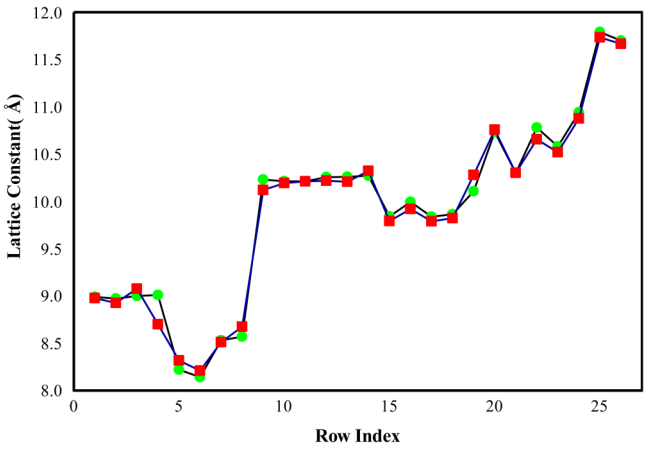

FIG. 4. Relationship between predicted and experimental values of lattice constants of the testing dataset.

matched with the experimental result during the training process. This is a clear indication that the algorithm successfully learned the functional dependency between the input parameters and the lattice constant values for different A_2XY_6 cubic crystals.

This assumption is validated by testing the algorithm's performance on a new dataset (testing data), which was not used in the training data. Figure 4 reflects the model's performance on the testing dataset. There is a high degree of agreement between the predicted and experimental values, which is similar to those obtained in the training phase of the algorithm. This result proves that the proposed model is capable of predicting experimental lattice constants of A_2XY_6 cubic crystals.

As previously mentioned, there are linear regression-based models that have been used to predict the lattice constants of cubic crystals. For example, Brik and Kityk[13] proposed a simple linear equation shown in Eq. (7) for prediction of the lattice constant,

$$a = 1.96325(R_A + R_X) + 0.98102(R_X + R_Y) + 0.07593(\chi_Y - \chi_X) + 0.57901. \quad (7)$$

TABLE VI. Comparison of SVR prediction and Brik's model for prediction of the lattice constant of cubic crystals of the form A2XY6 (A = K, Cs, Rb, Tl; X = tetravalent cation; Y = F, Cl, Br, I).

									Relative deviation	
	R_A	R_X	R_Y	X_A	χ_X	Expt. result	SVR pred.	Brik model	SVR pred.	Brik model
Cs_2GeF_6	1.880	0.530	1.330	0.790	2.010	8.990	8.976	8.855	0.014	0.135
Cs_2MnF_6	1.880	0.530	1.330	0.790	1.550	8.972	8.926	8.890	0.046	0.082
Cs_2PdF_6	1.880	0.615	1.330	0.790	2.200	9.000	9.076	8.924	0.076	0.076
K_2HfF_6	1.640	0.710	1.330	0.820	1.300	9.010	8.700	8.615	0.310	0.395
K_2MnF_6	1.640	0.530	1.330	0.820	1.550	8.221	8.318	8.419	0.097	0.198
K_2SiF_6	1.640	0.400	1.330	0.820	1.900	8.142	8.210	8.265	0.069	0.123
Rb_2MnF_6	1.720	0.530	1.330	0.820	1.550	8.531	8.511	8.576	0.020	0.045
Rb_2PdF_6	1.720	0.615	1.330	0.820	2.200	8.570	8.675	8.610	0.105	0.040
Cs_2GeCl_6	1.880	0.530	1.810	0.790	2.010	10.230	10.119	10.206	0.111	0.024
Cs_2IrCl_6	1.880	0.625	1.810	0.790	2.200	10.212	10.193	10.285	0.019	0.073
Cs_2MoCl_6	1.880	0.650	1.810	0.790	2.160	10.212	10.211	10.313	0.001	0.101
Cs_2ReCl_6	1.880	0.630	1.810	0.790	1.900	10.255	10.218	10.313	0.037	0.058
Cs_2SeCl_6	1.880	0.500	1.810	0.790	2.550	10.260	10.207	10.136	0.053	0.124
Cs_2TaCl_6	1.880	0.680	1.810	0.790	1.500	10.271	10.322	10.392	0.051	0.121
K_2ReCl_6	1.640	0.630	1.810	0.820	1.900	9.840	9.791	9.842	0.049	0.002
K_2TaCl_6	1.640	0.680	1.810	0.820	1.500	9.994	9.920	9.921	0.074	0.073
Rb_2MnCl_6	1.720	0.530	1.810	0.820	1.550	9.838	9.789	9.927	0.049	0.089
Tl_2MoCl_6	1.700	0.650	1.810	1.800	2.160	9.864	9.822	9.959	0.041	0.096
Tl_2TeCl_6	1.700	0.970	1.810	1.800	2.100	10.107	10.279	10.014	0.172	0.093
Cs_2WBr_6	1.880	0.660	1.960	0.790	1.700	10.733	10.757	10.784	0.024	0.051
K_2OsBr_6	1.640	0.630	1.960	0.820	2.200	10.300	10.302	10.245	0.002	0.055
K_2TeBr_6	1.640	0.970	1.960	0.820	2.100	10.780	10.656	10.586	0.124	0.194
Rb_2SnBr_6	1.720	0.690	1.960	0.820	1.960	10.580	10.519	10.479	0.061	0.101
Rb_2UBr_6	1.720	0.890	1.960	0.820	1.700	10.940	10.877	10.695	0.063	0.245
Cs_2PoI_6	1.880	0.940	2.200	0.790	2.000	11.790	11.734	11.720	0.056	0.070
Cs_2TeI_6	1.880	0.970	2.200	0.790	2.100	11.700	11.665	11.741	0.035	0.041
Total deviation									1.757	2.704

Table VI compared the results obtained from the support vector regression model proposed and Eq. (7). Equation (7) exhibits a better prediction in only 5 out of the 26 samples considered. Meanwhile, the SVR model showed higher prediction accuracy in 21 out of the 26 samples considered. In summary, the total deviation for the SVR model and Eq. (7) are 1.757 and 2.704, respectively. This clearly revealed the high prediction performance of the proposed SVR model over the linear equation for the prediction of the lattice constant of A_2XY_6 crystals.

IV. CONCLUSION

In this study, we proposed the application of the support vector regression (SVR) algorithm for the modeling of the lattice constants of A_2XY_6 cubic crystals (A = K, Cs, Rb, TI; X = tetravalent cation; Y = F, Cl, Br, I) as a better alternative to linear empirical models. The SVR model presented in this work was developed using simple atomic information: ionic radii and electronegativity of the constituent elements as model inputs. The optimization of the SVR model parameters was done via the Bayesian optimization algorithm. In total, 85 experimental datasets were used in this study; out of this, 59 datasets (70% of the total) were used for training the SVR algorithm and the remaining 29 datasets (30% of the total) were used for validation of the prediction accuracy of the proposed model. Based on the testing dataset, the SVR model predictions were compared with the linear empirical model in the literature to evaluate its performance accuracy. For the 29 datasets, the SVR model and the empirical model has a total deviation of 1.757 and 2.704, respectively. Clearly, the SVR model exhibits better accuracy and is thus recommended as a better approach for the estimation of the lattice constant of cubic crystalline structures. This study also revealed that the ionic radii are more important as model inputs than electronegativities; however, both are needed in order to obtain a higher accuracy in the prediction of lattice constants of the A_2XY_6 cubic crystals (A = K, Cs, Rb, TI; X = tetravalent cation; Y = F, Cl, Br, I).

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