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MATERIALS OF ELECTRONIC ENGINEERING

Predictions of Chalcospinels with Composition $ABCX_4$ (X = S or Se)

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Abstract—New chalcospinels of the most common compositions were predicted: $A^IB^{III}C^{IV}X_4$ (X = S or Se) and $A^{II}B^{III}C^{III}S_4$ (A, B, and C are various chemical elements). They are promising for the search for new materials for magneto-optical memory elements, sensors, and anodes in sodium-ion batteries. The parameter "*a*" values of their crystal lattice are estimated. When predicting, only the values of the properties of chemical elements were used. The calculations were carried out using machine learning programs that are part of the information-analytical system developed by the authors (various ensembles of algorithms of the binary decision trees, the linear machine, the search for logical regularities of classes, the support vector machine, Fisher linear discriminant, the k-nearest neighbors, the learning a multilayer perceptron, and a neural network) for predicting chalcospinels not yet obtained, as well as an extensive family of regression methods, presented in the scikit-learn package for the Python language, and multilevel machine learning methods that were proposed by the authors for estimation of the lattice parameter value of new chalcospinels. The prediction accuracy of new chalcospinels according to the results of the cross-validation is not lower than 80%, and the prediction accuracy of the parameter of their crystal lattice (according to the results of calculating the mean absolute error when cross-validation in the leave-one-out mode) is ±0.1 Å. The effectiveness of using multilevel machine learning methods to predict the physical properties of substances is shown.

Keywords: chalcospinel, crystal lattice parameter, prediction, machine learning

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INTRODUCTION

A unique combination of magnetic, optical, and semiconductor properties makes chalcogenide spinels promising for creation of magneto-optical memory and sensor elements [1–7]. The possibility of using these substances as anodes in sodium-ion batteries was shown [8]. Application of simple chalcospinels does not meet the requirements of contemporary electronics; thus, studies devoted to obtaining and researching spinels more complicated in composition are carried out [1, 3, 9, 10]. However, the literature contains information about a small range of synthesized multicomponent spinels. In particular, the most complete information about them can be found in the Phases database on the properties of inorganic compounds [11], prepared by us, which reflects data on less than 80 quaternary spinels with sulfur and selenium of various compositions.

The aim of this work is to predict new spinels of composition $ABCX_4$, where A, B, and C are different chemical elements and X is S or Se.

ANALYSIS OF EXISTING METHODS FOR PREDICTING NEW SPINELS

The Phases database [11] contains information about 28 spinels of composition $ABCS_4$ and 5 of composition $ABCSe_4$ (Table 1). In most cases, these compositions correspond to solid solutions.

Taking practical importance of chalcospinels into account, multiple attempts to find criteria of their formation, including properties of chemical elements in their composition, were made [21–32]. In the vast majority of cases, these criteria referred to three-component chalcospinels of composition AB_2X_4.

In [21, 22], it was proposed to use projections in coordinates $K_{AB} = \frac{\chi_A \cdot \chi_B}{r_e^2} - \frac{r_A}{r_B}$, where χ_A and χ_B are the electronegativities of elements A and B, $r_e^2 = (r_A + r_X)^2 + (r_B + r_X)^2 + 1.155(r_A + r_X)(r_B + r_X)$, where r_A, r_B, and r_X are the ionic radii of the corresponding ions of elements A, B, and X, in order to separate domains of existence of various crystallographic structures of substances of composition AB_2X_4. In article [23], it was proposed to use for these purposes projec-

Table 1. Known chalcospinels

Composition	Link	Composition	Link	Composition	Link
$LiInSnS_4$	[10]	$CuInSnS_4$	[13]	$CuCoRhS_4$	[15]
$CuVTiS_4$	[12, 13]	$AgCrSnS_4$	[15]	$CdSbInS_4$	[18]
$CuCrSnS_4$	[12–14]	$AgInZrS_4$	[14]	$ZnCrGaS_4$	[19]
$CuCrTiS_4$	[13, 14]	$AgInSnS_4$	[3]	$HgCrGaS_4$	[19]
$CuCoTiS_4$	[13]	$CuCrVS_4$	[3]	$CdCrInS_4$	[20]
$CuTiZrS_4$	[13]	$CuCrRhS_4$	[14, 16]	$ZnCrInS_4$	[20]
$CuTiSnS_4$	[13]	$MnCrInS_4$	[16]	$CuCrSnSe_4$	[14]
$CuVZrS_4$	[13]	$FeCrInS_4$	[16]	$CuCrTiSe_4$	[14]
$CuVSnS_4$	[13]	$CoCrInS_4$	[16]	$CuCrZrSe_4$	[14]
$CuCrZrS_4$	[12–14]	$NiCrInS_4$	[17]	$CuCrHfSe_4$	[14]
$CuCrHfS_4$	[14]	$CdCrGaS_4$	[17]	$AgCrSnSe_4$	[14]

tions in coordinates of ionic radii r_A and r_B; projections in coordinates of pseudo-potential radii were proposed in [24, 25]; and ionic radii according to Shannon–Prewitt of elements A and B were used to separate inverse and normal chalcospinels in [24]. Diagrams in coordinates of pseudo-potential orbital radii were used in [26–28] for determination of stability domains of chalcospinels. Projection in coordinates "sum of ionic radii by Shannon–Prewitt– sum of electronegativities of A, B, and X" was applied in [29] for classification of chalcogenide substances of composition AB_2X_4 with various types of crystal lattice. Ionic radii by Shannon–Prewitt [30] and ratios of ionic radii [31] were used to search for the limits of existence of the main structural families of the aforementioned composition.

In [32], new chalcogenide substances of composition AB_2X_4 with various types of crystalline lattice were predicted on the basis of quantum-mechanical computations.

Analysis of various projections of points corresponding to different classes of substances of composition $ABCX_4$ allows making a conclusion that the use of only dimensional factors and electronegativities is not enough for formation of criteria which allow reliably predicting new chalcospinels of the aforementioned composition. It is necessary to include other properties of chemical elements into the sought criteria as well. Exactly such an approach was suggested by us for predicting chalcospinels of composition AB_2X_4 [33, 34]. The use of the method of machine learning [35] allowed forming criteria which include a number of parameters of the components (electronegativities, ionization potentials, covalent radii, and other properties of the elements, as well as thermodynamic properties of simple chalcogenides). These criteria provided the possibility to predict not yet obtained chalcogenide substances of composition AB_2X_4 and the type of their crystal structure at room temperature and atmospheric pressure [33, 34]. Experimental verification of the obtained predictions showed that their average accuracy was higher than 78%. An attempt to use a machine learning program based on the method of potential functions in [36] was less successful. According to experimental verification, the accuracy of predictions was below 37%.

METHODOLOGY

In order to solve the formulated problem, we applied our developed information-analytical system (IAS) [37], which unites databases on properties of inorganic substances and materials with a subsystem of information analysis and search for multidimensional regularities based on machine learning methods. The procedure of using the IAS for searching for complicated regularities in chemical information and predicting of new inorganic phases as well as estimation of their properties included the following stages:

(1) Selection of examples for computer-aided analysis;

(2) Selection of the initial set of properties of elements for formation of the sought criteria;

(3) Searching for properties of elements and simple algebraic functions of these properties which would provide the greatest separation of various classes of phases of the aforementioned composition;

(4) Computer-aided analysis of the selected information with further selection of machine learning algorithms which would allow forming criteria providing the best separation of different classes of substances;

(5) The use of found multidimensional criteria for predicting not yet obtained phases and estimating their properties.

Let us consider the methodology of application of the IAS for predicting chalcospinels of composition $ABCX_4$ at different stages in more detail.

(I) Selection of examples for computer-aided analysis

The main source of the initial information for computer-aided analysis was the Phases database [11] as part of IAS. The most widespread compositions were selected: $A^IB^{III}C^{IV}X_4$ (X = S or Se) and $A^{II}B^{III}C^{III}S_4$. In the second case of machine learning, data on triple substances of composition $A^{II}B^{III}_2S_4$ were added to the selection for analysis, which allowed increasing the accuracy of further prediction.

(II) Selection of the initial set of properties of components for formation of the sought criteria

Information about substances is represented in computer memory in the form of a matrix whose rows included the set of values of parameters of elements in a specific substance with indication to which class it belongs. Selection of the initial properties of elements is based on existing concepts of physical and chemical nature of the researched substances. Information about properties of elements is obtained from our developed database Elements (http://phases.imet-db.ru/elements). The first two stages resulted in formation of selection of set for further computer-aided analysis (learning sample).

(III) Finding of the most important properties of elements and simple algebraic functions of these properties for classification

The properties of elements and automatically generated algebraic functions of these properties which are the most significant for separation of different classes of substances were selected using a special software package [38] included in IAS. The use of algebraic functions of properties of elements simplifies further formation of the sought criteria. It is necessary to note that addition of such functions significantly increases the number of parameters of components (to hundreds and even thousands), which also increases the dimension of the feature space. Thus selection of only the most significant algebraic functions for further inclusion in the sought criterion substantially accelerates the process of its formation and often promotes increased prediction accuracy. The package [38] results in finding parameters which separate the given classes of substances in the best possible way.

(IV) Computer-aided analysis of the selected information

Criteria making it possible to predict new chalcospinels were sought using a complex of 15 machine learning programs [35, 39] as part of IAS [37]. The applied programs made it possible to distinguish domains in multidimensional space of properties of components which correspond to known compounds with spinel structure. The accuracy of predicting taking the formed criteria into account was estimated using the widely applied common procedure of cross-validation, which is described in detail in [39]. As a result, the most accurate machine learning algorithms were selected for solving the given problem. In order to compensate errors of separate machine learning algorithms and to obtain a more accurate solution, we applied the procedure of collective decision making based on special packages [39] included in IAS. The accuracy of generalized criteria obtained using these packages was estimated using test detection of information about the given amount of substances, data on which was randomly selected from learning samples and was not used in machine learning (at the final stage of prediction, these test cases were returned back to the sample for machine learning). It is necessary to note that the use of collective methods is a good way to increase prediction accuracy and is widely applied in various areas [40].

(V) Prediction of not yet obtained chalcospinels

When predicting new chalcospinels, we used only data on the properties of elements. All the predictions are for atmospheric pressure and room temperature. The procedure of prediction and formation of prediction tables is carried out in IAS automatically. The user specifies only sets of symbols of elements.

All the mentioned procedures of machine learning and prediction were performed separately for compositions $A^IB^{III}C^{IV}X_4$ (X = S or Se) and $A^{II}B^{III}C^{III}S_4$.

COMPUTATION

Composition $A^IB^{III}C^{IV}X_4$ (X = S or Se)

After expert evaluation, the sample for computer analysis included information on 20 chalcospinels of composition $A^IB^{III}C^{IV}X_4$ and 103 compounds with a crystal structure other than spinel under normal conditions, as well as 10 systems $A_2X–B_2X_3–CX_2$ which do not form compounds of composition $ABCX_4$.

Composition $A^{II}B^{III}C^{III}S_4$

Information about 13 chalcospinels of composition $A^{II}B^{III}C^{III}S_4$ and 20 compounds with a crystal structure different from spinel under normal conditions was selected in the sample for machine learning. The learning sample also contains examples of 48 spinels of composition $A^{II}B^{III}_2S_4$, 90 compounds of this composition with a crystal structure other than spinel, and 18 $AS–B_2S_3$ systems in which compounds of composition AB_2S_4 are not formed.

In both problems, the initial set of parameters of components includes the following properties of chemical elements: covalent radius (by Bokii–Belov), pseudopotential radius (by Zunger), ionic radius (by Shannon–Prewitt), distances to core (S6) and valence electrons (S5) (by Schubert), first, second and third ionization potentials of atoms (E5, E6, E7), numbers (by Mendeleev–Pettifor) (M1–M11), quantum num-

Table 2. Prediction of a spinel crystal structure type in compounds of composition $A^IB^{III}C^{IV}X_4$

X	S								Se							
A^I	Cu				Ag				Cu				Ag			
$C^{IV}B^{III}$	Ti	Zr	Sn	Hf	Ti	Zr	Sn	Hf	Ti	Zr	Sn	Hf	Ti	Zr	Sn	Hf
Ti		#S	#S	S		#A	A	A		A	A	A		A	A	A
V	#S	#S	#S	S	A	S	S	S	A	S	S	S	A	A	A	A
Cr	#S	#S	#S	#S	#A	#A	#S	S	#S	#S	#S	#S	#A		#S	S
Co	#S	S	S	S	A	S	S	S	S	S	S	S	A	S		S
In	S	S	#S	S	S	#S	#S	S		A	#A			A	#A	

ber (A5), electronegativity (by Pauling), chemical potential of Miedema, temperatures of melting and boiling, standard entropy, atomization enthalpy, thermal conductivity, molar heat capacity (I10), etc.—in total, 123 values for each system A–B–C– X (composition $A^IB^{III}C^{IV}X_4$) and 96 values of each system A–B–C–S (composition $A^{II}B^{III}C^{III}S_4$). The values of these properties were obtained from our developed database Elements (http://phases.imet-db.ru/elements).

RESULTS AND DISCUSSION

Predicting Chalcospinels of Composition $A^IB^{III}C^{IV}X_4$ (X = S or Se)

Analysis of the learning sample using the package [38] showed that functions S5(B)*S5(X) and M2(B)/A5(A) possess the highest separating capability, where M2(B) is the number of element B by Mendeleev–Pettifor (H t-d start right). However, analysis of location of points on projection (whose coordinates are the aforementioned most significant algebraic functions) shows that domains corresponding to chalcospinels, compounds with crystal structures different from spinel structure, and systems without formation of compounds of the predicted composition strongly intersect. Nevertheless, addition of the values of these algebraic functions to the initial properties of chemical elements allowed achieving 96% accuracy of test prediction using machine learning programs based on methods of "binary decision trees," "linear machine," and "formation of logical regularities" [39] and applied majority vote for making collective decisions.

Criteria formed during machine learning allowed predicting new chalcospinels. Table 2 presents a part of the obtained results. The following notation is accepted hereinafter: S—prediction of spinels; A—prediction of compounds with crystal structure different from spinel; empty cells—undefined result. Sign "#" marks earlier studied systems, information about which is used when forming multidimensional criteria. All the predictions are given for room temperature and atmospheric pressure.

Predicting sulfospinels of composition $A^{II}B^{III}C^{III}S_4$

Analysis of projections of points in coordinates of algebraic functions of properties of chemical elements (E6(A)*E7(B) and I10(A)+I10(B)) which are the most important for distinguishing the domain of stability for spinel structure found using package [38] showed that they are insufficient for good separation of compounds of different classes. Moreover, addition of these functions to the initial parameters of chemical elements did not change the accuracy of test prediction (81%). Thus, only the initial properties of elements were used for formation of classification criterion.

New chalcospinels were predicted using an ensemble of machine learning programs [39] based on methods of support vector machine, Fischer linear discriminant, k-nearest neighbors, learning of multilayer perceptron, and neural network using the complex committee method—averaging. Table 3 presents a part of the obtained prediction results. For notation, see Table 2.

Predicting the Parameter of Crystal Lattice of Chalcospinels

Presently, the parameters of the crystal lattice of compounds is predicted using machine learning methods [41–43].

Estimation of the parameters of the crystal lattice of the predicted chalcospinels included several stages:

(1) Selection of the initial set of properties of elements for formation of learning samples.

The learning sample with information about known chalcospinels is represented in the form of a matrix whose rows include the set of parameter values of elements in a specific substance with indication of the value of parameter "*a*" of cubic crystal lattice of spinels. The set of properties of elements included dimensional factors (covalent radius (by Bokii-Belov), pseudopotential radius (by Zunger), ionic radius (by Shannon-Prewitt), distances to core and valence electrons (by Schubert), electronegativity (by Pauling), temperatures of melting and boiling, first, second, and third ionization potentials of atoms—in total, 11 values

Table 3. Prediction of a spinel crystal structure type in compounds of composition $A^{II}B^{III}C^{III}S_4$

C	Ga								In							
A B	Mn	Fe	Co	Ni	Cu	Zn	Cd	Hg	Mn	Fe	Co	Ni	Cu	Zn	Cd	Hg
Cr	A	A	A	A	S	#S	#S	#S	#S	#S	#S	#S	S	#S	#S	S
Mn		A	A	A	S	A	S	S		S	S	S	S	S	S	S
Co		S		S	S	S	S	S		S		S	S	S	S	S
Rh	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S
Ir	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S

of properties for each element in composition of chalcospinel. This stage resulted in two learning samples for further computer-aided analysis for various compositions: $A^{I}B^{III}C^{IV}X_4$ (X = S or Se) (19 examples) and $A^{II}B^{III}C^{III}S_4$ (53 examples, including information about spinels of composition $A^{II}B^{III}_2S_4$).

(2) Computer-aided analysis of the selected information with further selection of the best algorithms.

Values of the parameters of the crystal lattice were predicted using the widespread software package scikit-learn [44] as well as multilayer methods of machine learning [45]. Prediction accuracy was determined by the results of computation of mean absolute error (MAE) and mean squared error (MSE) (in cross-validation regime leave-one-out).

For illustrating the possibilities of the used methods (with the least values of errors), Table 4 presents the results of prediction for the parameter of the crystal lattice of the studied chalcospinels of composition $A^{I}B^{III}C^{IV}X_4$. The best results were obtained using ridge regression, Bayes ridge regression [46], and regression of automatic relevance determination [47], as well as a multilayer approach representing a combination of machine learning methods using algorithms of random forest construction [48] and elastic net [49]. Figure 1 shows the results of prediction using the latter combined approach graphically. It is necessary to note that such a multilayer approach provided the least errors of prediction (Table 4). Table 5 presents results of prediction using this method.

The results of prediction of the lattice parameter of sulfospinels of composition $A^{II}B^{III}C^{III}S_4$ presented in Table 6 and graphical illustration of these results (Fig. 2) allow selecting a multilayer method which represents a combination of machine learning methods using "random forest" and "elastic net" for predicting unknown values of parameter "*a*" (Table 7).

CONCLUSIONS

The efficiency of using machine learning when designing new inorganic substances was shown.

These methods provided successful prediction of not yet obtained chalcospinels of composition $ABCX_4$ and estimation of values of parameter "*a*" of their crystal lattice. Only values of properties of chemical elements were used for prediction. Computations were

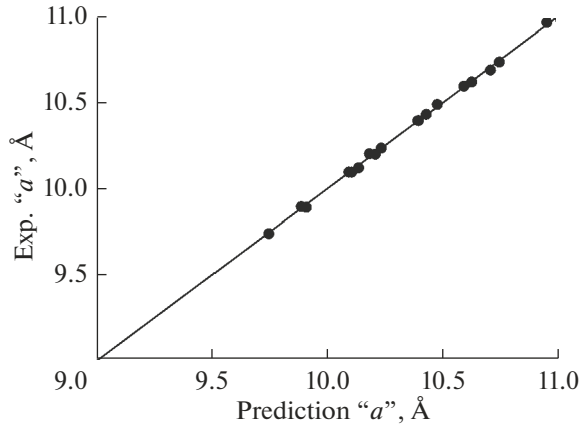

Fig. 1. Comparison of the predicted values of the crystal lattice parameter of chalcospinels with composition $A^{I}B^{III}C^{IV}X_4$ with experimental data using multilevel prediction ("random forest" + "elastic net").

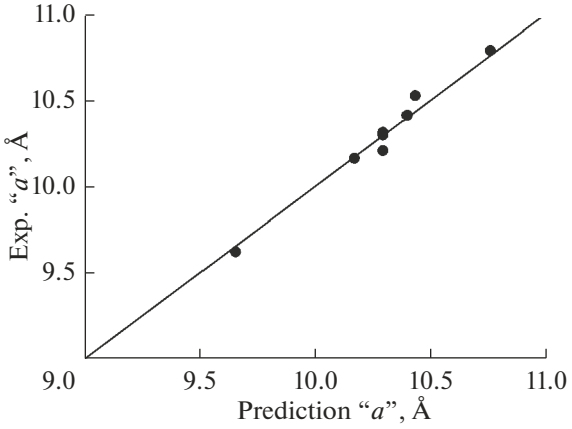

Fig. 2. Comparison of the predicted values of the crystal lattice parameter of chalcospinels with composition $A^{II}B^{III}C^{III}X_4$ with experimental data using multilevel prediction ("random forest" + "elastic net").

Table 4. The results of the examination prediction of the crystal lattice parameter of chalcospinels with composition $A^{I}B^{III}C^{IV}X_4$

Composition	MAE	0.10	0.10	0.11	0.09
	MSE	0.02	0.02	0.02	0.01
	method	Ridge Regression	Bayesian Ridge Regression	ARD Regression	Random Forest + Elastic Net
	a, Å experiment	*a*, Å prediction			
$LiInSnS_4$	10.629	10.63	10.63	10.61	10.63
$CuVTiS_4$	9.902	9.91	9.91	9.91	9.91
$CuCrSnS_4$	10.2	10.17	10.17	10.17	10.21
$CuCrTiS_4$	9.9	9.90	9.90	9.90	9.89
$CuCoTiS_4$	9.744	9.75	9.75	9.75	9.750
$CuTiZrS_4$	10.236	10.22	10.22	10.21	10.24
$CuTiSnS_4$	10.244	10.25	10.25	10.24	10.24
$CuVZrS_4$	10.209	10.15	10.15	10.15	10.19
$CuVSnS_4$	10.124	10.19	10.19	10.19	10.14
$CuCrZrS_4$	10.1	10.13	10.13	10.14	10.11
$CuCrHfS_4$	10.1	10.10	10.10	10.10	10.10
$CuInSnS_4$	10.4938	10.48	10.48	10.49	10.48
$CuCrSnSe_4$	10.7	10.67	10.67	10.68	10.71
$CuCrTiSe_4$	10.4	10.40	10.40	10.40	10.40
$CuCrZrSe_4$	10.6	10.64	10.64	10.64	10.60
$CuCrHfSe_4$	10.6	10.60	10.60	10.60	10.60
$AgCrSnS_4$	10.44	10.44	10.44	10.44	10.43
$AgInSnS_4$	10.74	10.75	10.75	10.76	10.75
$AgCrSnSe_4$	10.97	10.95	10.95	10.95	10.96

Table 5. Prediction of the crystal lattice parameter of chalcospinels with composition $A^{I}B^{III}C^{IV}X_4$

Composition	*a*, Å	Composition	*a*, Å	Composition	*a*, Å
$CuInTiS_4$	10.10	$AgCoZrS_4$	10.19	$CuCoZrSe_4$	10.46
$CuCoZrS_4$	9.99	$AgInZrS_4$	10.62	$CuVSnSe_4$	10.48
$CuInZrS_4$	10.41	$AgVSnS_4$	10.40	$CuCoSnSe_4$	10.43
$CuCoSnS_4$	9.95	$AgCoSnS_4$	10.22	$CuVHfSe_4$	10.52
$CuTiHfS_4$	10.23	$AgVHfS_4$	10.37	$CuCoHfSe_4$	10.46
$CuVHfS_4$	10.17	$AgCrHfS_4$	10.25	$AgCoZrSe_4$	10.71
$CuCoHfS_4$	9.98	$AgCoHfS_4$	10.17	$AgCrHfSe_4$	10.79
$CuInHfS_4$	10.39	$AgInHfS_4$	10.59	$AgCoHfSe_4$	10.70
$AgInTiS_4$	10.35	$CuCoTiSe_4$	10.26		
$AgVZrS_4$	10.40	$CuVZrSe_4$	10.53		

Table 6. The results of the examination prediction of the crystal lattice parameter of chalcospinels with composition $A^{II}B^{III}C^{III}S_4$

Composition	MAE	0.18	0.17	0.18	0.10
	MSE	0.05	0.04	0.05	0.02
	method	Ridge Regression	Bayesian Ridge Regression	ARD Regression	Random Forest + Elastic Net
	a, Å experiment	*a*, Å prediction			
$MnCrInS_4$	10.4297	10.42	10.42	10.42	10.41
$FeCrInS_4$	10.323	10.30	10.30	10.30	10.31
$CoCrInS_4$	10.31	10.26	10.25	10.29	10.31
$NiCrInS_4$	10.22	10.15	10.16	10.20	10.31
$CdCrGaS_4$	10.1784	10.22	10.24	10.24	10.18
$CuCoRhS_4$	9.64	9.65	9.66	9.67	9.66
$CdSbInS_4$	10.8	10.78	10.77	10.783	10.77
$CdCrInS_4$	10.54	10.51	10.51	10.49	10.44

Table 7. Prediction of the crystal lattice parameter of chalcospinels with composition $A^{II}B^{III}C^{III}S_4$

Composition	*a*, Å	Composition	*a*, Å	Composition	*a*, Å
$CuCrVS_4$	9.92	$ZnRhGaS_4$	9.96	$NiRhInS_4$	10.22
$CuCrRhS_4$	9.90	$ZnIrGaS_4$	9.96	$NiIrInS_4$	10.23
$ZnCrGaS_4$	10.12	$CdMnGaS_4$	10.19	$CuCrInS_4$	10.35
$HgCrGaS_4$	10.19	$CdCoGaS_4$	9.94	$CuMnInS_4$	10.37
$ZnCrInS_4$	10.40	$CdRhGaS_4$	10.02	$CuCoInS_4$	10.22
$MnRhGaS_4$	9.91	$CdIrGaS_4$	10.02	$CuRhInS_4$	10.23
$MnIrGaS_4$	9.92	$HgMnGaS_4$	10.18	$CuIrInS_4$	10.24
$FeCoGaS_4$	9.78	$HgCoGaS_4$	9.94	$ZnMnInS_4$	10.41
$FeRhGaS_4$	9.89	$HgRhGaS_4$	10.03	$ZnCoInS_4$	10.27
$FeIrGaS_4$	9.90	$HgIrGaS_4$	10.03	$ZnRhInS_4$	10.28
$CoRhGaS_4$	9.83	$MnRhInS_4$	10.29	$ZnIrInS_4$	10.29
$CoIrGaS_4$	9.84	$MnIrInS_4$	10.33	$CdMnInS_4$	10.46
$NiCoGaS_4$	9.75	$FeMnInS_4$	10.33	$CdCoInS_4$	10.32
$NiRhGaS_4$	9.85	$FeCoInS_4$	10.21	$CdRhInS_4$	10.32
$NiIrGaS_4$	9.86	$FeRhInS_4$	10.21	$CdIrInS_4$	10.36
$CuCrGaS_4$	9.97	$FeIrInS_4$	10.24	$HgCrInS_4$	10.43
$CuMnGaS_4$	9.93	$CoMnInS_4$	10.33	$HgMnInS_4$	10.44
$CuCoGaS_4$	9.73	$CoRhInS_4$	10.21	$HgCoInS_4$	10.30
$CuRhGaS_4$	9.83	$CoIrInS_4$	10.23	$HgRhInS_4$	10.31
$CuIrGaS_4$	9.84	$NiMnInS_4$	10.34	$HgIrInS_4$	10.34
$ZnCoGaS_4$	9.88	$NiCoInS_4$	10.22		

carried out with application of an information-analytical system based on methods of machine learning and software packages of the scikit-learn system.

According to data of test prediction using cross-validation, the prediction accuracy of new chalcospinels was not lower than 80% and that of the parameter of their crystal lattice was ±0.1 Å.

The efficiency of using multilevel methods of machine learning for predicting physical properties of substances was shown.

The predicted chalcospinels are promising in the search for new materials to create magneto-optical elements of memory and sensors, as well as anodes in sodium-ion batteries.

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