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Computer-Aided Design of New Inorganic Compounds with Composition ABX_2 (X = S, Se, Te)

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Abstract—Chalcogenide compounds of the ABX_2 (X = S, Se, Te) composition is a promising class of semiconductor materials. Materials for solar batteries were developed on the basis of chalcopyrites of the $CuInS_2$, $CuInSe_2$, and $CuGaSe_2$ structures [1–5]. The compound $AgSbSe_2$ is a promising thermoelectric material for use at average temperatures (350–600°C) [6]. However, nonlinear-optical applications of chalcogenides with the general formula ABX_2 are the most interesting [6–13]. In connection with the prospect of practical use of the compounds of this structure, it is obviously important to design their unstudied analogs.

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METHODS

The problem of designing new inorganic compounds can be formulated as follows [14]: find a set of chemical elements and their ratio (i.e., qualitative and quantitative structure) for the creation (under set external conditions) of certain spatial molecular or crystal structure of the compound, allowing the necessary functional properties to be realized. The initial information for calculations should be only properties of the chemical elements and data on other compounds already studied. Thus, the question is to search for dependences between the properties of systems (for example, properties of compounds) and properties of the elements forming these systems.

Several *approaches* to the solution of problems of computer-aided design [14] are known: the quantum-chemical approach, the simple empirical 2D and 3D criteria of the formation of compounds with set properties, and multivariate empirical classifying principles intended for the prediction of new inorganic substances.

The quantum-chemical approach to calculate chemical compounds is based on the Schrödinger equation, whose exact solution for certain inorganic substances is connected with serious mathematical difficulties which managed to be overcome only for simple systems. Currently used approximations do not always allow calculation of new multicomponent compounds from first principles.

Development of empirical criteria of formation of compounds with set properties uses the vast amount information on inorganic substances and also is based on the existence of periodic dependences between the properties of compounds and their elements. Empirical criteria are a model of these periodic dependences, and their pursuit is carried out on the basis of well-studied substances. Developed criteria can be used for designing new inorganic compounds, analogs of existing substances.

As a rule, simple empirical criteria (e.g., the well-known rules of Hume–Rothery, Laves, and Mathias and the Goldschmidt tolerance factor) include two or three properties of components and consequently are fairly rough since parameters of inorganic compounds, especially multicomponent, are defined by many properties of the elements. Therefore, the development of this approach was the conversion to multivariate dependences. Searching for these classifying rules is possible using various computer programs for data analysis. In this case, it is possible to include any number of properties of components or their functions, which relieves the developer of criteria from the labor-intensive process of selecting the initial parameters. Thus, the program for data analysis can exclude those properties which do not influence the classification. An important advantage of this approach is the possibility of correcting the obtained rule because of new experimental data not matching the old criterion. Thus, the computer approach offered by us [14] transforms the process of development of empirical classifying rules from a problem whose solution is carried out mainly by well-qualified experts into a technology suitable for all researchers.

Programs for data analysis based on algorithms of computer training for image recognition are the most effective for chemical applications. The task of the computer training is formulated as follows. Let the space of properties of elements be set. It is known that it contains a fixed number of areas with uncertain boundaries, and there are no rules for determining the attachment of points to one area or another. During the computer system training, points from these areas (learning sample) are shown and the information to what area these points belong is given. The purpose of

Table 1. Properties of elements used for the description of ABX_2

No.	Property	No.	Property
1	Pseudopotential radius (by Canger)	15	Third ionization potential (I_3)
2	Regular number (by Mendeleev–Pettifor)	16	Miedema chemical potential (only for *A* and *B*)
3	Distance to internal electrons (by Schubert)	17	Group number (only for *A* and *B*)
4	Distance to valence electrons (by Schubert)	18	Electronegativity (by Pauling)
5	Quantum number	19	Heat conduction
6	Melting point	20	Molar heat capacity
7	Boiling point	21	Solid body entropy
8	Ionic radius (by Bokii and Belov)	22	Debye temperature (only for *A* and *B*)
9	Evaporation enthalpy	23	$(R_{covA} - R_{covB})/R_{covC}$
10	Melting enthalpy	24	$(I_{1A} - I_{1B})/I_{1C}$
11	Atomization enthalpy	25	$(I_{2A} - I_{2B})/I_{2C}$
12	Covalent radius (R_{cov})	26	$(I_{3A} - I_{3B})/I_{3C}$
13	First ionization potential (I_1)	27	$(X_A - X_B)/X_C$, (X is electronegativity by Martynov–Bacanov)
14	Second ionization potential (I_2)	28	Formal valence (only for *A* and *B*)

training is to construct surfaces which partition not only the available points but also all other points belonging to these areas. Thus, the initial information for the computer analysis is a matrix, each line of which corresponds to a well-known compound (or chemical system), represented in the computer as a set of values of the component properties (chemical elements or simple compounds) with the indication of the class to which the compound belonged. The multivariate criterion generated during the computer analysis also includes only the properties of components. Therefore, for the prediction of the class to which a new compound belongs, it is necessary to know only the values of properties of its components.

For automation of the search for multivariate classifying principles and prediction of characteristics of new inorganic compounds, we have developed a special information-analytical system (IAS) [15]. It contains an integrated system of databases (DBs) on properties of inorganic compounds and materials created at the Baikov Institute of Metallurgy and Materials Science [14, 16] and a package of programs for computer training for image recognition. On the basis of long-term testing of programs for computer training, we selected the most effective methods for image data recognition [17, 18]: the system RECOGNITION, which was developed by the Computing Center of the Russian Academy of Sciences [17], and the system for computer training to process the formation of concepts ConFor, developed in the Institute of Cybernetics, National Academy of Science of Ukraine [18]. The developed IAS is intended for designing new inorganic compounds on the basis of computer analysis of information databases.

This work contains the results obtained by using the IAS for designing new inorganic compounds of the ABX_2 structure (*A* and *B* are different chemical elements; X = S, Se, or Te).

COMPUTER-AIDED DESIGN OF NEW COMPOUNDS OF THE ABX_2 COMPOSITION

The first studies on predicting the formation of ABX_2 (X = S, Se or Te) were done at the end of the 1970s [19]. Then the new data were used to retrain the computer [20]. An experimental check of more than three hundred predictions obtained in these works [19, 20] showed that the average error of prediction of the formation of ABX_2 was 11%, and the error of prediction of phases with the crystal structure of the type α-$NaFeO_2$ was 15% [14].

The purpose of the present research was the specification of predictions for the formation of the chalcogenide-containing compounds ABX_2 using new experimental data on the existence of compounds of this structure, as well as the prediction of the crystal structure type of these compounds under ambient conditions. In comparison with the earlier works [19, 20], where the computer training and prediction of unknown compounds was done separately for sulfides, selenides, and tellurides, the possibilities of IAS allowed information analysis for all chalcogenides of the predicted structure to be conducted simultaneously and also a wider set of properties of the chemical elements *A*, *B*, and *X* to be considered (Table 1).

1. Prediction of Formation of ABX_2 Compounds under Ambient Conditions

Data on 667 examples of the formation of ABX_2 (X = S, Se, or Te) and 504 examples of the absence of compounds of this structure in the systems A_2X–B_2X_3 and AX–BX under ambient conditions were used for the computer training. The data were taken from the DB on the properties of inorganic compounds "Phases" [14, 21, 22]. Properties of the elements A, B, and X (Table 1), whose values were taken from the DB "Elements" [22], were used for the uploading of compounds into the computer memory.

For the analysis of data, several algorithms of computer training were used [17]. Quality of the training was estimated on the basis of examination recognition, which was carried out on a material of the training sample in two modes: without and with sliding control. In the first case, objects of the training sample were estimated after the computer training. However, this way of evaluating the training quality and the subsequent prediction is extremely unreliable. Therefore, the second way of evaluating the training quality was used. In the latter case, the given part (f) of objects was withdrawn from the training sample. The computer training was carried out on the remaining objects, and the withdrawn objects were presented for recognition. The number of errors was fixed. Then the "control" objects were returned to the training sample and other objects were withdrawn, and the procedure was repeated until all objects of the training sample had been used control ones. This procedure allows one to estimate the accuracy of algorithms of recognition for a certain training sample more objectively, especially in the case of the methods of recognition for which the undesirable effect of "retraining," when the algorithm is "adjusted" only for the training sample, is observed and subsequently shows poor results during the prediction of new objects. After the end of training with sliding control, the average error of recognition, which is used further for choosing the best algorithms for the collective decision, is calculated.

Decision making on the existence of a compound with the application of the strategy of collective methods [17] allows the reliability of prediction to be increased. The idea of this approach consists in the following. First of all, different algorithms for image data recognition are used independently for the prediction of new compounds. Then the results obtained by using different algorithms are processed in a certain way [17] and the final collective decision on the reference of compounds to a certain class is formed. In this case, the errors of predictions obtained by various algorithms are mutually compensated, which leads to a more exact result.

The simplest collective method is voting of the predictions, where the result that is most often given out by the various algorithms is chosen. However, the voting of predictions does not always allow improving the reliability of prediction for complicated tasks, especially in the case of weak execution of the basic hypothesis for image data recognition—a hypothesis of compactness of objects in the space of properties. Therefore, we have also used other methods for collective decisions, such as the convex stabilizer, Woods dynamic method, Bayes method, logic correction of sets of recognizing algorithms, areas of competence, and patterns of decision making [17]—methods intended for the solution of complicated tasks of prediction.

The analysis of the training results using various algorithms has shown that the best predictions under sliding control have been obtained for the binary decision tree method (accuracy of prediction being 72%), formation of logic laws (accuracy of prediction being 67.3%), and voting under deadlock tests (accuracy of prediction being 67.6%). These algorithms have been used for collective decisions using the committee method, in which the resulting prediction is calculated as an average arithmetic value of predictions obtained using different algorithms [17].

2. Prediction of the Crystal Structure Type of ABX_2 Compounds under Ambient Conditions

Data on 158 examples of the formation of ABX_2 (X = S, Se, or Te) with the crystal structure under ambient conditions (298 K and 1 atm) α-$NaFeO_2$ (space group $R3(-)m$), 44 compounds with NaCl structure (space group $Fm3m$), 47 compounds with chalcopyrite structure (space group $I4(-)2d$), and 24 compounds with TlSe structure (space group $I4/mcm$) were used for the computer training. The data were taken from the DB on the properties of inorganic compounds "Phases" [14, 21, 22]. Properties of the elements A, B, and X (Table 1), whose values were taken from DB "Elements" [3], were used for the uploading of compounds into computer memory.

The problem was solved in two ways. In the first case, multiclass training and prediction, where the cumulative information on the four above-mentioned crystal phases was used, was applied. In the second case, four problems of the dichotomy were solved—division into two classes, e.g., class 1, compounds with chalcopyrite crystal structure, and class 2, compounds with other structure. The results of predictions were compared, and a decision was made if the predictions obtained by multiclass prediction and dichotomy did not contradict each other. The results are summarized in Tables 2–5.

Several methods for the computer training were used to analyze the data [17]. The examination recognition was carried out on material of the training sample in two modes: without and with sliding control. Methods that showed the best results for the examination recognition were used for the collective decisions.

Tables 2–5 contain the results of prediction of the possibility for the formation and type of crystal struc-

Table 2. Prediction of the formation and crystal structure of compounds in the systems A_2X–B_2X_3 under the ambient conditions

Element *B*	Element *A* at *X*																							
	S								Se								Te							
	Li	Na	K	Cu	Rb	Ag	Cs	Tl	Li	Na	K	Cu	Rb	Ag	Cs	Tl	Li	Na	K	Cu	Rb	Ag	Cs	Tl
B	#5	#5	#5	3	#5	3	#5	#5	1	1		#5	1	3	1	4	1	1	4		1		1	4
Al	#5			#3		#3		4	#5	#4	#5	#3		#3		#5		#4	#4	#3		#3	4	#4
P			5	#5		#5	5	#5	2	1	1	#5	1		5	#5	2		4	3	5		5	4
Sc	#1	#1	1	#5	1			#1	1	1	1		1	#5	1		1		1		1		1	
Ti	#5	#1	#1		#5			#4	#5	#1	1	3	1	3	5	#4		4	4		5	3	5	4
V	#5	#1	1		1				#5	#1	1	3	#5	3	5		#5	#5			5		5	4
Cr	#5	#1	#1	#5	#1	#5		#5	2	#1	1	#5	#1	#5	5				5	3	5	#5	5	#5
Mn	5		1		1				#5	#5	1		#5	3	5		#5	#5	#5		#5	#5	#5	
Fe	#5		#5	#3	#5	#3		#5		1	#5	#3	#5	#3		#5			1	#3	1	#3	1	5
Co	5								2	1	1	3	1	3	5	5	2			3	5	5	5	
Ni	5	1		#5						#2	1		1	#5	5				1	3	5	#5	5	
Ga	#5	#5	#5	#3	#5	#3	5	#5	5	4	#5	#3	4	#3		#5	#3	#4	#5	#3		#3		#4
As		#5		#5		#5	5	#5		#5	#5	#5	#5	#2	#5	5	2		4	#6	5	#2	5	
Y	#2	#1	#1	5	1	#5	5	#1	#1	#1	1		1	#5	1	#1	1	1		#5	1	#5	1	#1
Mo	#5	1	1						2	1	1	3	1	3	5	5			4	3	5		5	
Rh		1	1	3					2		1	3	1	3	5		2		4	3	5	3	5	
In	#5	#1	#5	#3	#5	#3	#5	#4	#5	#1	5	#3	#5	#3		#4	#3	#4	#4	#3		#3	4	#4
Sb		5	#5	#5	#5	2	5	2	2	5	#5	#5	#5	#2		5	#2	#2	4	#5	#5	#2	#5	#1
La		#2	#1		#1		#1	#6	#5	#1	1	#5	#1		1	#6	2		1		1		1	6
Ce		#2	#1	#5	#1		#1	#6	#5	#1	1	#5	#1	#6	1	#6			1		1		1	#6
Pr	#2	#1	#1	#5	#1		#5		1	#1	1	#5	#1	#6	1	#1	2		1	#5	1		1	#1
Nd	#2	#1	#1	#5	#1		#5			#1	1		#1		1	#1	1	1	1	#5	1		1	#1
Pm		1	1	5	1	5		1	1	1	1		1		1	1	1	1			1		1	
Sm	#2	#1	#1	#5	#1	#5	#5	#1		#1	1	#5	#1	#6	1	1		1	1		1		1	#1
Eu	#2	#1	#1	#5	#1	#5	#5	#1		#1	1	#5	1	#6	1	#6		1	1		1		1	
Gd	#2	#1	#1	#5	#1	#5	#5	#1	#1	#1	1	#5	#1	#5	1	#1	1	1	1		1	#5	1	#1
Tb	#2	#1	#1	#5	#1	#5	#5	#1	#1	#1	1	#5	#1		1	#1	1	1			1	5	1	#1
Dy	#2	#1	#1	#5	#1	#5	#5	#1	#1	#1	1		1	#5	1	#1	1	1			1	#5	1	#1
Ho	#1	#1	#1	#5	#1	#5	#5	#1	#1	#1	1		#1	#5	1	#1	1	1			1	#5	1	#1
Er	#1	#1	#1	#5	#1	5	#5	#1	#1	#1	1		#1	#5	1	#1	1	1	#1		1	#5	1	#1
Tm	#1	#1	#1	#5	#1	#5	#5	#1	1	1	1		1	#5	1	#1	1	1			1	#5	1	#1
Yb	#1	#1	#1	#5	#1	#5	#5	#1		#1	#1		1	#5	#5	1	2	1	1	#5	1		1	
Lu	#1	#1	#1	#5	#1	#2	#5	#1	1	1	1		#1	#5	1	#1	1	1			1	#5	1	#1
Tl	2		#5	#3	#5	3	#5			#4	#4	#3	4	#3				4	4	#3	4	#3		4
Bi	#2	#2	#2	#5	#1	#1		#1	#2	#2	#2	#2	#5		#5	#2	#2	#2		#5		1		#1
Th	2	1	1		1		1	1	1	1	1		1		1	1	1	1	4		1		1	4
Pa	2	1	1		1		1	1	1	1	1		1		1	1	1	1			1		1	
U			1		1		5	1			1		1		5						5		5	
Np					1			1	1	1	1		1		1				4		1		1	4
Pu	2		1		1			1	1	1	1		1		1	1			4		1		1	

Table 3. Prediction of the formation and crystal structure of compounds in the systems *A*S–*B*S under ambient conditions

Element *B*	Element *A*																																
	Be	Mg	Ca	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	Sr	Pd	Ag	Cd	Sn	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Tb	Dy	Ho	Er	Tm	Yb	Lu	Hg	Pb
Mg	6																																
Ca	6	6																															
Mn	6	6	6																														
Fe	6	#6	#6	#6																													
Co	6	6	6	6	#6																												
Ni			6	6																													
Cu	6		6	6			#5																										
Zn	#5	6	#6	#6	#6	6		#6																									
Ga				6			3	#3	3																								
Ge	6	6	6	6	#6	6		#5	6	6																							
Sr	6	6	6	6	#6	6					6																						
Pd		6	6	#6			#5	3	6			6																					
Ag	6	6	6	6	6	6		3	6	6	#6	6	6																				
Cd	6	#6	6	#6	6	6	6		#6	6	6	6	6	#6																			
Sn	6	6	#6	6	#6	6	6		6	6	6	6	6		#6																		
Ba		5	6	#5	5	#5	#5		#5		5	6	#5		#5	5																	
La				6	6	6				#6	6		6		6																		
Ce		6		6	6	6		5	6	6	6		6		6	6		6															
Pr				6	6	6		5	6		6		6		6																		
Nd				6	6	6		5			6		6																				
Pm		6		6	6	6	6		6	6	6		6		6	6		6	6	6	6												
Sm		#6	#6	6	6	6	6	5	6	#6	6	#6	6	5	6		#6	#6	6	6	6	6											
Eu	6	#6	#6	6	6	6	6	5	6		6	#6	6	5	6	6	#6	6	6	6	6	6	6										
Gd								5	6			1		5			1				#1												
Tb								5						5			1																
Dy								5	6					5			1																
Ho								5						5			1																
Er								5						5			1																
Tm								5	6		6			5	6	6	1		6	6				6									
Yb								5	6		6			5	#6	6																	
Lu								5				1		2	6		1																
Hg	6	6		6	6	6			#6		#6				#6	#6	#5												6				
Pb	6	6	6	6	#6	6	6		6	#6	6	6	6		6	#2		6	6	6	6	6	6	6	6	6	6	6	6	6	6	#6	
Ra	6	6	6	6	6	6			6	6	6	6	6		6	6		6	6	6	6	6	6	6					6	6	6	6	6
U		6	#5								6	#5			6		#5		6	#6				6						6		6	6
Np															6																	6	
Am									6						6	6																6	

Note: In Tables 2–5, the following designations were used: 1—prediction of the structure of the α-$NaFeO_2$ type; 2—prediction of the structure of the NaCl type; 3—prediction of the structure of the chalcopyrite type; 4—prediction of the structure of the TlSe type under the ambient conditions (298 K and 1 atm); 5—prediction of the structure distinct from the ones mentioned above; 6—prediction of the absence of ABX_2; the symbol # is used for objects for the computer training; empty entries indicate discrepancies of predictions using different collective methods or uncertain prediction.

Table 4. Prediction of the formation and crystal structure of compounds in the systems *A*Se–*B*Se under ambient conditions

Element *B*	Element *A*																																		
	Be	Mg	Ca	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	Sr	Pd	Ag	Cd	Sn	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Hg	Pb	U
Ca	6	6																																	
Mn		6	6																																
Fe		6	6	#6																															
Co		6	6	6	6																														
Ni	6	6	6	6	6	6																													
Cu		6	6	6	6	6	6																												
Zn	#6	6	6	#6	6	6	6	6																											
Ga				6	6	6		#3																											
Ge		6	6	6	6	6	6	6	3	#6																									
Sr	6	6	6	6	6	6	6	6	6		6																								
Pd	6	6	6	6	6	6	6		6		6	6																							
Ag	6	6	6	6	6	6	6		6	6	#6	6	6																						
Cd	6	#6	6	#6	6	6	6		6	#6	#6	6	6	6																					
Sn	6	6	6	6		6	6		#6	#6	#6	6	6		#6																				
Ba	6	6		6	6	6	6	6	6		6		6	6	6	6																			
La	6		6	6	6	6	6	#5	6		6																								
Ce	6	6	6	6	6	6	6	#5	6		6		6	6	6	#6																			
Pr	6		6	6	6	6	6	#5	6	6	6			6		#6																			
Nd	6			6	6	6	6		6		6				6	#6			6																
Pm	6		6	6	6	6	6	6	6	6	6					6																			
Sm	6		6	6	6	6	6	#5	6		6			6		#6					#6	6													
Eu	6	6	6	6	6	6	6	#5	6		6		6	6	6	6		6	6	6	6	6	6												
Gd				6	6	6		#5	6		6			#5	6	#6	1						#2												
Tb			6					#5			6					#6																			
Dy			6								6			#5		#6																			
Ho			6						6		6			#5		#6																			
Er			6								6			#5		#6		#2	6																
Tm	6		6	6	6	6	6		6		6			#5		6			6																
Yd	6		6	6	6	6	6	6	6		6			#5		#6		2		#2															
Lu				6	6	6	6		6		6			#5		6			6			6									6				
Hg	6	6	6	6	6	6	6	6	#6		#6	6	6	6	#6	#6		6	6	6	6	6	6		6					6	6	6			
Pb	6	#6	6	#6				6	#6	#6	#6	6	6	#6	#6	#6	6	6	6	6	6	6	6	6		6	6	6	6	6	6	6	#6		
Ra	6	6	6	6	6	6	6	6	6		6	6	6	6	6	6			6														6		
U		6	6	6	6	6	6		6		6				6	6		6	6	6	6	6		6	6	6					6	6	6	6	
Np				6	6	6	6				6		6		6	6		6	6	6	6	6			6	6						6		6	6
Am		6	6	6	6	6	6	6	6		6		6		6	6			6						6					6	6		6	6	

Table 5. Prediction of the formation and crystal structure of compounds in the systems *A*Te–*B*Te under ambient conditions

Element *B*	Element *A*																																		
	Be	Mg	Ca	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	Sr	Pd	Ag	Cd	Sn	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Hg	Tl	Pb
Ca	6	6																																	
Mn		6	6																																
Fe		6	6	#6																															
Co		6	6	6	6																														
Ni	6	6	6	6	6	6																													
Cu		6	6	6	6	6	6																												
Zn	#6	6	6	#6	6	6	6	6																											
Ga				6	6	6	#6	#3	#3																										
Ge		6	6	#6	6	#6	6	#6	#6	#5																									
Sr	6	6	6	6	6	6	6	6	6		6																								
Pd	6	6	6	6	6	6					6	6																							
Ag	6	6	6	6	6	6		#5			#6	6	6																						
Cd	6	#6	6	#6	6	6	#6		#6	#3	#6	6	6	#6																					
Sn	6	6	6	#6	6	#6	6	#6	#6	#5	#6	6	6	#5	#6																				
Ba	6	'6	6	6	6	6	6	6	6		6		6	6	6	6																			
La	6	6	6	6	6	6	6		6		6		6		6	6																			
Ce	6	6	6	6	6	6	6		6		6		6	6	6	6																			
Pr	6	6		6	6	6	6	5	6		6		6		6	6			6																
Nd	6	6		6	6	6	6	5	6		6		6		6	6			6																
Pm	6	6	6	6	6	6	6	6			6		6		6	6			6																
Sm	6	6		6	6	6	6		6		#6		6		6		6		6		6	6													
Eu	6	6		6	6	6	6	6	6		6		6	6	6			6	6	6		6	6												
Gd	6	6		6	6	6			6		6			5	6	6			6																
Tb	6			6	6						6				6	6			6			6													
Dy											6			5	#6	6		6	6			6													
Ho	6	6	6	6	6	6	6				6			5	6	6		6	6			6													
Er											6			5		#5			6			6													
Tm	6	6	6	6	6	6	6				6	6	6	5	6	6		6	6	6	6	6	6	6						#6					
Yd	6	6	6	6	6	6	6	5	6	#6	#6		6		6				6			6	6		6					#6					
Lu	6	6	6	6	6	6	6				6		6	#	6	6			6			6								6	6				
Hg	6	#6	6	6	6	6	6	6	#6	#3	#6	6	6	6	#6	#6		6	6	6	6	6	6	6	6	6				6	6	6			
Pb	6	#6	6	#6	#6	6	#6	6	#6	#6	#6	6	6	#6	#6	#6	6	#6	6	6	6	6	6	#6	6	6	6	6	6	#6		6	#6	#6	
Ra	6	6	6	6	6	6	6	6	6		6	6	6	6	6	6																	6		6
U	6	6	6	6	6	6	6		6		6				6	#6		6	6	6				6							6		6		#6
Np	6			6	6	6	6		6		6		6		6	6																	6		6
Am	6	6	6	6	6	6	6	6	6		6		6		6	6									6					6	6		6		6

ture of ABX_2 that were obtained by comparison of the results of application of the best methods for the computer training and the collective decision making.

CONCLUSIONS

Using methods for computer training to recognize image data, design of hundreds of new compounds of the ABX_2 structure (A and B are different chemical elements; X = S, Se, or Te) was carried out with various types of crystal structures promising for seeking new materials for electronics.

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