APPLICATION OF ARTIFICIAL INTELLIGENCE METHODS TO COMPUTER DESIGN OF INORGANIC COMPOUNDS

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Abstract: In this paper the main problems for computer design of materials, which would have predefined properties, with the use of artificial intelligence methods are presented. The DB on inorganic compound properties and the system of DBs on materials for electronics with completely assessed information: phase diagram DB of material systems with semiconducting phases and DB on acousto-optical, electro-optical, and nonlinear optical properties are considered. These DBs are a source of information for data analysis. Using the DBs and artificial intelligence methods we have predicted thousands of new compounds in ternary, quaternary and more complicated chemical systems and estimated some of their properties (crystal structure type, melting point, homogeneity region etc.). The comparison of our predictions with experimental data, obtained later, showed that the average reliability of predicted inorganic compounds exceeds 80%. The perspectives of computational material design with the use of artificial intelligence methods are considered.

Keywords: artificial intelligence, computer design of materials, databases on properties of inorganic materials, information-analytical system.

ACM Classification Keywords: I.2.1 Artificial Intelligence: Applications in Chemistry

Introduction

Now the search for new inorganic materials is carried out, for the most part, on the basis of the experience and intuition of researchers. The problem of *a priori* prediction of compounds that have not yet been synthesized and evaluations of their properties is one of the most difficult problems of modern inorganic chemistry and materials science. Here the term "*a priori* prediction" means predicting yet unknown substances with predefined properties from only the properties of constituent components - chemical elements or more simple compounds.

The problem of predicting new compounds can be reduced to the analysis of the multidimensional array of the property values and the column vector of the desired property. Each row corresponds to some known chemical system, whose class is indicated by the row position of the column vector. For example, the multidimensional array can include the properties of chemical elements for set of known chemical systems with formation or without formation of compound with predefined composition (desired property). The process of analyzing all this information allows finding the classifying regularity. By substituting the values of the properties of the elements for unknown chemical system into the regularity thus found, it is possible to determine the class (compound formation or non-formation). So, the problem of *a priori* prediction of new compounds can be reduced to the classical task of computer learning. The chemical foundations of material computer design are based on Mendeleev's law which asserts that the periodic nature of changes in the properties of chemical systems depends on the nature and properties of the elements which makes these systems (compounds, solutions, etc). Another premise justifying the proposed approach is the existence of good classification schemes for inorganic substances.

Databases on Properties of Inorganic Materials and Substances as a Foundations of Material Computer Design

The application of computer learning methods for finding regularities is rather put into use in case of complete and qualitative initial data. Our experience of computer learning applications to chemistry shows that the number of erroneous predictions varies proportionally with ratio of number of errors in experimental data to number of learning set to be processed and the reliability of prediction grows with an increase of initial data volume (reliability mounts to a limit with an increase of size and representatives of learning set). Consequently, the application of the computer learning methods to chemistry implies the use of databases (DBs), containing

extensive bulks of qualitative information, as a basis. With this aim in mind, we develop the DBs containing data with the qualified expert assessment. The most interesting of them are DBs on materials for electronics with completely assessed information [Kiselyova *et al.*, 2004] and an inorganic compound properties DB containing partially assessed information [Kiselyova, 2002; Kiseleva *et al.*, 1996]. These DBs are integrated. The all our DBs have Internet-access (http://www.imet-db.ru).

1. A phase diagram DB of material systems with semiconducting phases "Diagram" [Kiselyova *et al.*, 2004] contains information on physical and chemical properties of the intermediate phases and the most important Pressure-Temperature-Concentration phase diagrams of semiconducting systems evaluated by qualified experts. Now the DB contains detailed information on several tens of semiconducting systems.

2). DB on acousto-, electro-, and nonlinear optical properties "Crystal" [Kiselyova *et al.*, 2004] contains detailed information regarding substances of these types evaluated by experts. In addition, DB includes extensive graphical information about properties of the materials.

3). A DB on inorganic compound properties "Phases" [Kiselyova, 2002; Kiseleva *et al.*, 1996] contains information about thermo-chemical and crystal chemical properties on more than 41,000 ternary compounds taken from more than 13,000 publications. Some of the data have been assessed by materials experts. This DB is a main data source for material computer design.

On the one hand, the use of DBs increases the reliability of predicting inorganic substances, and, on the other hand, the application of artificial intelligence methods extends the capabilities of databases owing to the search for regularities in the known information and the use of these regularities for prediction of new substances not yet synthesized.

Artificial Intelligence Methods for Material Computer Design

The search for, and development of effective material computer design systems were aimed at the creation of more powerful programs capable of analyzing, on the one hand, very large arrays of experimental information, and, on the other hand, of allowing construction of multidimensional classified regularities under the conditions of small sets. Improvements in electronics allowed the development of systems for chemical applications with a user-friendly interface, working in real time, for example, [Gladun, 1995; Gladun *et al.,* 1995; Chen *et al.,* 1999; Chen *et al.,* 2002; Pao *et al.,* 1999]. The trend has been a transition from the simplest algorithms of pattern recognition [Gulyev *et al.,* 1973; Kutolin *et al.,* 1978; Savitskii *et al.,* 1968; Talanov *et al.,* 1981; Vozdvizhenskii *et al.*, 1973] toward more powerful methods based on the use of neural and semantic networks [Kiselyova, 1987, 1993a, 1993b, 2002; Kiselyova *et al*., 1998, 2000; Manzanov *et al*., 1987; Pao *et al*., 1999; Savitskii et al., 1979; Villars *et al*., 2001; Yan *et al*., 1994].

It must be pointed out that since there are very many aspects in the domain of the artificial intelligence no criteria for selecting the most suitable algorithm for a particular application were available. After testing many algorithms intended for computer learning applications we formulated the principal criteria of a choice of the programs of computer learning ensuring the most effective decision of chemical tasks:

- possibility of the analysis of the large data volumes;
- possibility of obtaining qualitative classifying regularities at the analysis of the small learning sets;
- automatic exception of properties, which are no important for classification;
- possibility of decision of problems in conditions of weak fulfillment of the principal hypothesis of pattern recognition - hypothesis of compactness;
- fast learning and predicting;
- possibility of analysis of properties with the gaps of some values;
- possibility of analysis of properties having a qualitative nature (e.g., color, type of incomplete electronic shell: s, p, d, or f);
- high accuracy at the decision of chemical tasks;
- convenient interface of the user.

Taking into account these criteria we fixed on the class of algorithms in which all classifying regularities to be found could be presented in the form of a Boolean expression [Gladun, 1995]. This system of concept formation represents information about known chemical systems like - growing pyramidal networks (GPNs). A pyramidal

network is an acyclic oriented graph having no vertices with one entering arc. If the processes of concept formation are determined in the network then the pyramidal network is designated as a growing one [Gladun, 1995]. GPN is built during the process of objects' input. Each object (chemical system) is put in as a set of values of the component properties with an indication of the class to which the system belongs. The nearby values of components' properties are united into one interval using a special program or the experience of a researcher. Concept formation process consists of the analysis of vertices in built network and the choice of those ones that are the most typical for each class [Gladun, 1995]. These vertices became the checking vertices. The resultant concepts (classifying regularities) can be stored in computer memory and printed or read out in the form of a learned GPN or an equivalent Boolean expression, which the values of the component properties make the variables. During the prediction process, the computer receives only the atomic numbers of the elements or designations of simple compounds, while the values of the properties of the appropriate elements or simple compounds are automatically extracted from the DB. They are substituted into the GPN and the researchers can easily obtain the necessary prediction.

Application of Artificial Intelligence to the New Inorganic Materials Computer Design

Using this approach we solved problems of the following types [Kiselyova, 1987, 1993a, 1993b, 2002; Kiselyova *et al*., 1998, 2000; Savitskii *et al.*, 1979]:

- prediction of compound formation or non-formation for binary, ternary and more complicated systems;
- prediction of the possibility of forming ternary and more complicated compounds of desired composition;
- prediction of phases with defined crystal structures;
- estimation of phase properties (critical temperature of transition to superconducting state, homogeneity region, etc.).

Shown in Table 1 is a part of the table illustrating predictions of the Heusler phases with composition $ABCu_2$ [Kiselyova, 1987]. These results were obtained in the process of searching for new magnetic materials. All 6 checked predictions agreed with the new experimental data.

Table 1. Part of a table illustrating the prediction of a crystal structure type resembling the Heusler alloys for compounds with the composition $ABCu_2$

A / B	Li	Be	Al	K	Sc	V	Cr	Fe	Co	Ni	Ga	Ge	Y	Nb	Mo	Ru	Rh	Pd
Zn			+									-	-	-	-	-	-	-
Ga	+	+		+	⊕	+	+	+	+	+		O						
In	+	+		+	©	+	+	+	+	+	+	+	©	+	+	+	+	+
Sn	O	-	O	-	-	-		⊕	⊕	⊕	-	-	-	↔	-	-	-	-
Lu	-	-		-	-	-	-	-	-	-		-	-	-	-	-	-	-
Ta		-			-	-	-	-	-	↔		-	-	↔	-	-	-	-
Au	-	-		-	-	-	-	-	-	-		-	-	-	-	-	-	↔
Tl												-						
Pb	-	-	O	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Designations:

+ formation of a compound with the composition AB_2Cu and a crystal structure type resembling the Heusler alloys is predicted;
– formation of a compound with a crystal structure type resembling the Heusler alloys is not predicted;
⊕ a compound with a crystal structure type resembling the Heusler alloys was synthesized and appropriate information was used in the computer learning process;
↔ formation of a compound with a crystal structure type resembling the Heusler alloys is known from experiment and appropriate information was used in the computer learning process;
© predicted formation of a compound with a crystal structure type resembling the Heusler alloys which is confirmed by experiment;
O predicted absence of a compound with a crystal structure type resembling the Heusler alloys which is confirmed by experiment; empty square - indeterminate result.

In Table 2 the comparison between the results after predicting the compounds with composition ABX_2 (A and B – various elements; X – S or Se) [Savitskii *et al.*, 1979] and the new experimental data. These compounds

were predicted in the process of the search for new semiconductors. Only two predictions were detected to be in error ($CsPrS_2$ and $TlEuSe_2$).

Table 3 shows the predictions of more complicated compounds - new langbeinites with composition $A_2B_2(XO_4)_3$ [Kiselyova *et al*., 2000]. These results are importance for searching for new electro-optical materials. Of 17 checked predictions, 12 agreed with the new experimental data.

Table 2. Part of a table illustrating the prediction of compounds with the composition $A^IB^{III}X_2$

X	S							Se							
A^I / B^{III}	Li	Na	K	Cu	Rb	Ag	Cs	Li	Na	K	Cu	Rb	Ag	Cs	Tl
B			©	©	©		©			+	©	+	+	+	⊕
Al			©	⊕	+	⊕	+	©	⊕	⊕	⊕	+	⊕	+	⊕
Sc	©	©	+	⊕	+	+	+	+	+	+	⊕	+	⊕	+	+
Ti	⊕	©	©	©	⊕	+	⊕	©	©	+	+	+	+	+	+
V	⊕	©	+	+	+	+	+	©	©	+	+	+	+	+	+
Cr	⊕	⊕	©	⊕	⊕	⊕	+	+	⊕	+	⊕	⊕	⊕	+	⊕
Mn	+	+	+	+	+	+	+	©	©	+	+	©	+	©	+
Fe	+	⊕	⊕	⊕	⊕	⊕	⊕	+	+	©	⊕	©	⊕	©	⊕
Co	+	+	+	+	+		+	+	+	+	+	+	+	+	©
Ni	+	+	+	⊕	+	+	+	+	©	+	+	+	©	+	+
Ga	⊕	©	©	⊕	©	⊕	©	+	+	⊕	⊕	+	⊕	©	⊕
As	+	⊕	©	⊕	+	⊕	+	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕
Y	©	⊕	©	⊕	+	©	+	©	©	+	⊕	+	⊕	+	©
Rh	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
In	©	⊕	⊕	⊕	⊕	⊕	⊕	©	©	⊕	⊕	©	⊕	+	⊕
Sb	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕	⊕
La	©	⊕	⊕	⊕	⊕	↔	⊕		⊕		⊕		↔		↔
Ce	©	⊕	⊕	⊕	⊕		⊕	©	⊕	+	⊕		↔	+	+
Pr	⊕	⊕	⊕	⊕	⊕		⊗	+	⊕	+	⊕	©	↔	+	©
Nd	⊕	⊕	⊕	⊕	⊕		+	©	⊕	+	⊕	©	↔	+	©
Pm	+	+	+	+	+	+	+	+	+	+	+	+	-	+	+
Sm	⊕	⊕	⊕	⊕	⊕	⊕	+	©	⊕	+	⊕	©	↔	+	⊕
Eu	⊕	⊕	⊕	⊕	⊕	⊕	+	+	⊕	+	⊕	+	↔	+	⊗
Gd	⊕	⊕	⊕	⊕	⊕	⊕	+	©	⊕	+	⊕	©	©	+	⊕
Tb	⊕	⊕	⊕	⊕	©	⊕	+	©	⊕	+	⊕	©	⊕	+	©
Dy	⊕	⊕	⊕	⊕	©	⊕	+	©	⊕	+	⊕	+	⊕	+	©
Ho	⊕	⊕	⊕	⊕	©	⊕	+	©	⊕	+	⊕	©	⊕	+	©
Er	⊕	⊕	⊕	⊕	©	⊕	+	©	⊕	+	⊕	©	⊕	+	©
Tm	⊕	⊕	⊕	⊕	©	⊕	+	+	+	+	⊕	+	⊕	+	©
Yb	⊕	⊕	⊕	⊕	©	⊕	+	+	+	+	⊕	+	⊕	+	⊕
Lu	⊕	⊕	⊕	⊕	©	©	+	+	+	+	⊕	©	⊕	+	©
Tl	+	+	©	⊕	⊕	©	⊕	©		©	⊕	⊕	⊕	+	

Designations:

\+ predicted formation of a compound with composition ABX_2; - - prediction of no formation of a compound with composition ABX_2;

⊕ compound ABX_2 is known to be formed and this fact is used in the computer learning process;

↔ compound ABX_2 is not known to be formed and this fact is used in the computer learning process;

© predicted formation of a compound with composition ABX_2 which is confirmed by experiment;

⊗ predicted formation of a compound with composition ABX_2 which is not confirmed by experiment; empty square - indeterminate result.

Predicted compounds were then searched for new magnets, semiconductors, superconductors, electro-optical, acousto-optical, nonlinear optical and other materials required for new technologies. The comparison of these predictions with the experimental data, obtained later, showed that average reliability of predicted compounds exceeds 80%.

Table 3. Part of a table illustrating prediction of a crystal structure type for compounds with the composition $A_2B_2(XO_4)_3$

X	S					Cr					Mo					W				
A / B	Na	K	Rb	Cs	Tl	Na	K	Rb	Cs	Tl	Na	K	Rb	Cs	Tl	Na	K	Rb	Cs	Tl
Mg	L¢	(L)	(L)	(*)	L	L	L©		L©	L©	K¢	(K)	(L)	(L)	(L)		↔	(L)	L©	L
Ca	(*)	(L)	L©	(L)	(*)			L	L	L	(*)	?	?	?	?	(*)	*	?	?	?
Mn	(*)	(L)	(L)	L	(L)	L		(L)	L©	L	K	↔	(L)	(L)	(L)					
Fe	*	L©	L©		(L)	L	K	L	L	L	K	K	?	?	?		K			
Co	(*)	(L)	L©		(L)	L	K	L	L	L		(K)	(L)	(L)	↔		K			
Ni	(*)	(L)	L©	L	L	L		L	L	L	K	(K)	(L)	(L)	(L)					
Cu	(*)		L	*	L	L	K	L	L	L	K	(K)	?	?	?		K			
Zn	*	(L)	L	*	L	L	K	L	L	L	↔	(K)	(K)	-	(K)		K¢			
Sr	(*)	?	?		(*)	*	*	?	?	?	(*)	?	?	?	?	(*)	*	*	*	*
Cd	(*)	(L)	(L)		(L)							K	↔	(L)	K¢	(*)		L	L	L
Ba	(*)		(*)	(*)	(*)	*	*				(*)		*	*	*	*	*			
Pb					*	(*)	*	*©	*	*	(*)	*©	(*)	*¢	*	(*)	*	(*)	(*)	*

Designations:

L formation of a compound with the langbeinite crystal structure type is predicted;

K formation of a compound with the crystal structure type $K_2Zn_2(MoO_4)_3$ is predicted;

– the crystal structure differing from those listed above is predicted;

(L),(K) a compound with corresponding type of crystal structure was synthesized and appropriate information was used in the computer learning process;

↔ a compound with the crystal structure differing from those listed above does not exist at normal conditions and this information was used in the computer learning process;

(*) a compound $A_2B_2(XO_4)_3$ is not formed and this fact was used in the computer learning process;

¢ predicted formation of a compound with this structure type which is not confirmed by experiment;

© predicted formation of a compound with this structure type which is not confirmed by experiment; empty square - indeterminate result.

Information-Analytical System for Materials Computer Design

The promising line of materials computer design is associated with development of information-analytical system [Kiselyova, 1993a, 2002]. This system is intended for data retrieval on known compounds, the prediction of new inorganic compounds, not yet synthesized, and the forecasting of their properties.

This system includes learning and predicting subsystems based on artificial intelligence methods - method of concept formation using growing network CONFOR [Gladun, 1995; Gladun *et al.,* 1995] and other methods of computer learning [http://www.solutions-center.ru]. For increasing reliability of predicting the voting of predictions, which were obtained using various algorithms and component property descriptions will be carried out. The information-analytical system employs also the databases on properties of inorganic compounds, described above, and a DB on chemical elements, a knowledge base, a conversational processor and monitor (Figure 1).

The *knowledge base* of information-analytical system stores the regularities already obtained for various classes of inorganic compounds. They can be use in the prediction of phases and estimation of the phase properties, unless the databases have no such information about the particular chemical systems. Rules in the knowledge base are represented, for example, in the form of growing pyramidal networks, neural networks, logical expressions, etc.

The *conversational processor* manages the conversation of the user with the information-analytical system. It provides an expert in the given application domain a dialog with the information-analytical system also.

In the future, the employment of a linguistic processor in the software or software-hardware support can be expected. It will allow the system to understand the problem-oriented language of the user.

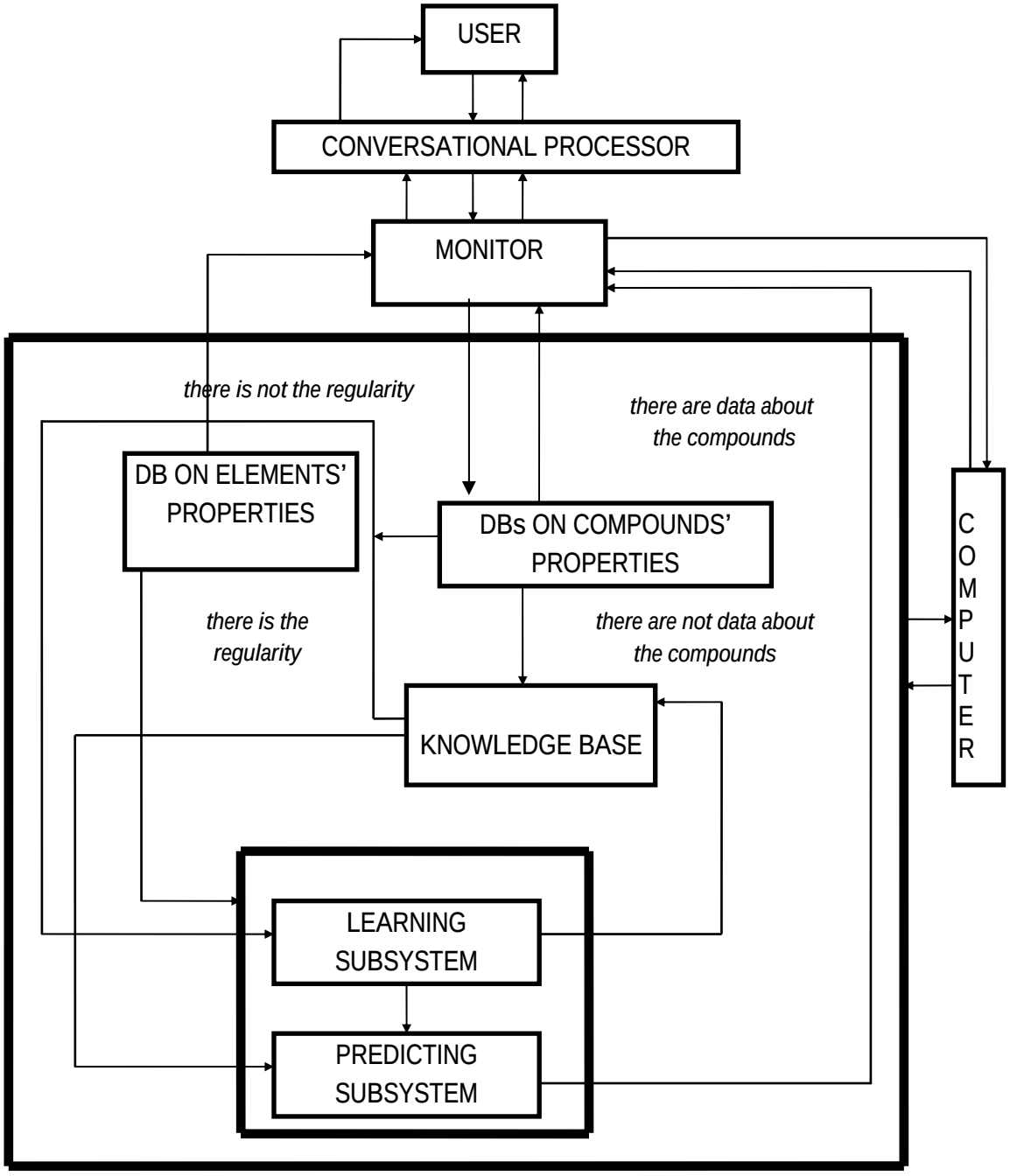

Figure 1. Schematic Diagram of an Information-Analytical System

The *monitor* controls the computation process and provides the interface between the functional subsystems as well as the Internet-access to the system. In addition, the monitor signals whenever new experimental data contradict existing classification regularities. Such contradictions will be eliminated by including the new data in the computer learning and modifying the regularity in the knowledge base.

The information-analytical system operates as follows (Figure 1). The user requests information about a compound of a certain composition. If data about this phase are stored in the databases, they can be extracted for user. If no information about the compound is stored in the databases, or if the information available is incomplete, the computer determines whether the regularity corresponding to the desired property for a compound of a certain type is present in the knowledge base. If the regularity is present, the databases supply the appropriate set of component properties for prediction of the desired characteristic. If the knowledge base does not have the desired regularity, then examples for the computer learning process are extracted from the databases. The correctness of these examples is estimated by the user once more; and, if the samples are found adequate for computer learning, the learning and prediction subsystems process them. The user receives the resultant prediction, while the new classifying regularity is stored in the knowledge base. The above example is the simplest of the problems that can be solved by an information-analytical system. A more complicated problem would be, for example, predicting all possible phases in ternary and multi-component systems, combined with the estimation of their properties. The previous problem can be solved by real-time processing. The latter problem requires much more time.

Conclusion

We have applied artificial intelligence methods for discovering regularities to the design of new inorganic materials. The effectiveness of the proposed approach is illustrated, for example, in Table 1, 2 and 3. The approach discussed in this paper for predicting new materials is based on a process, which is analogous to the search for new materials by an inorganic chemist. It has allowed predicting hundreds of new compounds in ternary, quaternary and more complicated chemical systems, not yet investigated. These compounds are analogs to known substances with important for industry properties. The predictions have been based on the interaction of growing pyramidal networks, computer learning and databases on properties of inorganic compounds. The proposed approach not only simulates the process of design of new inorganic materials but also extends the capabilities of the chemist in discovering new materials with powerful multi-dimensional data analysis tools.

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THE DISTRIBUTED SYSTEM OF DATABASES ON PROPERTIES OF INORGANIC SUBSTANCES AND MATERIALS

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Abstract: The principles of organization of the distributed system of databases on properties of inorganic substances and materials based on the use of a special reference database are considered. The last includes not only information on a site of the data about the certain substance in other databases but also brief information on the most widespread properties of inorganic substances. The proposed principles were successfully realized at the creation of the distributed system of databases on properties of inorganic compounds developed by A.A.Baikov Institute of Metallurgy and Materials Science of the Russian Academy of Sciences.

Keywords: database, distributed information system, inorganic substances and materials, reference database.

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