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Database on the Bandgap of Inorganic Substances and Materials

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Abstract—A database (DB) on the bandgap of inorganic substances available via the Internet (http://bg.imet-db.ru) was developed for the information service of specialists in the sphere of inorganic chemistry and materials science. The DB is integrated with other information systems on the properties of inorganic substances and materials, which provides the search of a wide range of parameters of a specific substance. The possibility of the use of the information from the developed DB for the search of relations between the bandgap width and other parameters of thermoelectric materials and for predicting the bandgap of chalcopyrites is considered.

Keywords: bandgap, inorganic substances, database, design of inorganic substances, pattern recognition
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INTRODUCTION

The bandgap E_g is a fundamental parameter of condensed phases, which characterizes the nature of chemical bonds in samples and the stability of crystal structures and explains the significant difference of physicochemical properties of substances.

Despite the importance of information on the bandgap for theoretical and practical materials science and numerous reference materials in this sphere, e.g., [1, 2], at present, there is no full computer database (DB) making it possible to operatively provide specialists with the data on this characteristic of solids. Among the available information resources, there is the AFLOWLIB.org DB developed at Duke University (USA) [3, 4], which includes the calculated information on E_g as one of the parameters of materials. On the website of the Physical-Technical Institute of the Russian Academy of Sciences, the data on the bandgap of chemical elements and the $A^{III}B^{V}$ compounds are presented [5]. However, a computer DB including the data on E_g for a wide range of inorganic substances and materials has not been developed so far.

The Bandgap DB, which is a part of an integrated database system (IDBS) on the properties of materials for electronics of IMET [6, 7], contains the experimental and calculated information on E_g for thousands of inorganic substances and materials of different compositions. Besides Bandgap, the IDBS includes the Diagram DB on the phase diagrams of semiconductor substances [8], the Crystal DB on the properties of acousto-optical, electro-optical, and nonlinear optical substances [9], the Phases DB on the properties of inorganic compounds [10], the Elements DB on the properties of chemical elements, and the AtomWork DB on the properties of inorganic compounds developed at the National Institute for Materials Science (Japan) [11].

The aim of this article is to describe the structure and operating regimes of the Bandgap DB by citing specific examples of the its use for the search and analysis of information on the properties of inorganic substances and materials and for the prediction of the bandgap of inorganic compounds.

STRUCTURE, SOFTWARE, AND WORKING REGIMES OF THE BANDGAP DB

The values of the bandgap of solids are determined by the chemical composition of a substance and by the crystal and defective structure of a sample. The E_g value depends on temperature, pressure, electric, magnetic, and gravitational fields, and other parameters. The conceptual structure of the Bandgap DB takes into account the above important characteristics of the subject domain. The database contains the information on the bandgap width of the basic classes of inorganic substances. It also contains the information on the methods of determining E_g (the Comments section) in different temperature intervals, chemical and phase compositions, crystal structures (crystal system, structure type, and space group), and orientations of samples at measurements. The basis of the DB are the E_g values determined by various experimental methods (optical, thermal, and electrophysical) at normal measurement conditions (room temperature, atmospheric pressure, and absence of external electric and magnetic fields). The accuracy of determination of E_g values by the experimental methods is $\delta E_g \sim 0.1$ eV (sometimes ~0.01 eV), which is sufficient for a

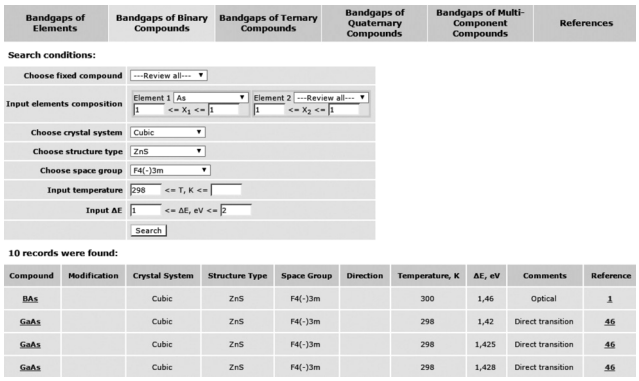

Fig. 1. The menu for the search of information in the DB.

detailed classification of compounds [12]. For all the data, the literature references are given.[1] The database includes the graphic information on the band structure, the dependences of the bandgap on various factors, etc. The calculated data on the E_g value are also provided. In the theoretical calculations of the band structure, the results obtained by quantum theory methods (the linear combination of atomic orbitals, the orthogonalized plane waves, the pseudopotential, etc.) are used [13–16]. The accuracy of the theoretical calculations of E_g usually does not exceed ~0.5 eV.

The basis of the software is the relational DB managed by the Microsoft SQL Server 2008 developed in the form of a web-based application using the Active Server Pages technology. For the access to the data, the ActiveX Data Objects interface is used. The web-server is the Internet Information Server 7.0 based on the Microsoft Windows Server 2008 platform. The search of information in the DB is performed by the user's request using a specially developed menu (Fig. 1).

A request can include a composition of a substance, a crystal system, a crystal structure type, a space group of symmetry, an interval of temperatures, and E_g values.

Currently, the database contains the data on about 3000 substances (more than 5500 records). The information is presented in English. The open access to the information of the Bandgap DB is possible via the Internet (http://bg.imet-db.ru). For registration, users should enter the data concerning their professional status and interests, after which they obtain a login and a password for entry into the information system.

It is important that the Bandgap DB is integrated with other information systems, i.e., a user can simultaneously obtain fairly full information on a substance from various DBs of the IMET IDBS: on the phase diagram and crystal structure from the Diagram or the AtomWork DB; on the acousto-optical, electro-optical, and nonlinear optical properties from the crystal

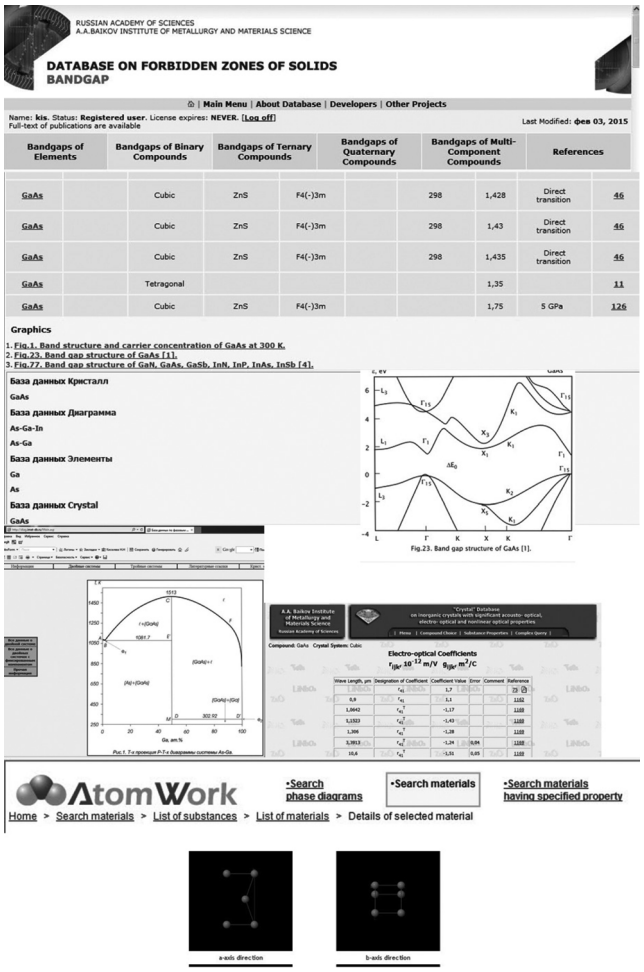

Fig. 2. Example of the presentation of consolidated information on the bandgap and other properties of the GaAs compound.

DB; etc. (Fig. 2). The integrated DBs provide significantly higher information capabilities.

The databases provide the information service for specialists and they are sources of data for the search for relations between the parameters of substances and other calculations.

SEARCH FOR RELATIONS BETWEEN THE BANDGAP AND THE PARAMETERS OF THERMOELECTRIC MATERIALS

Thermoelectric materials (TEM) (E_g = 0–1 eV) are characterized by the thermoelectric figure of merit $ZT = \alpha^2\sigma T/\kappa$, which is related to efficiency of thermoelectric energy converters, where α is the Seebeck coefficient; σ and $\kappa = \kappa_L + \kappa_e + \kappa_b$ are the specific electrical conductivity and thermal conductivities, respectively; κ_L, κ_e, and κ_b are the lattice, electronic, and bipolar components of the thermal conductivity, respectively; and T is the absolute temperature [12].

[1] Because of licensing restrictions, the full texts of publications are available only to staff members of IMET.

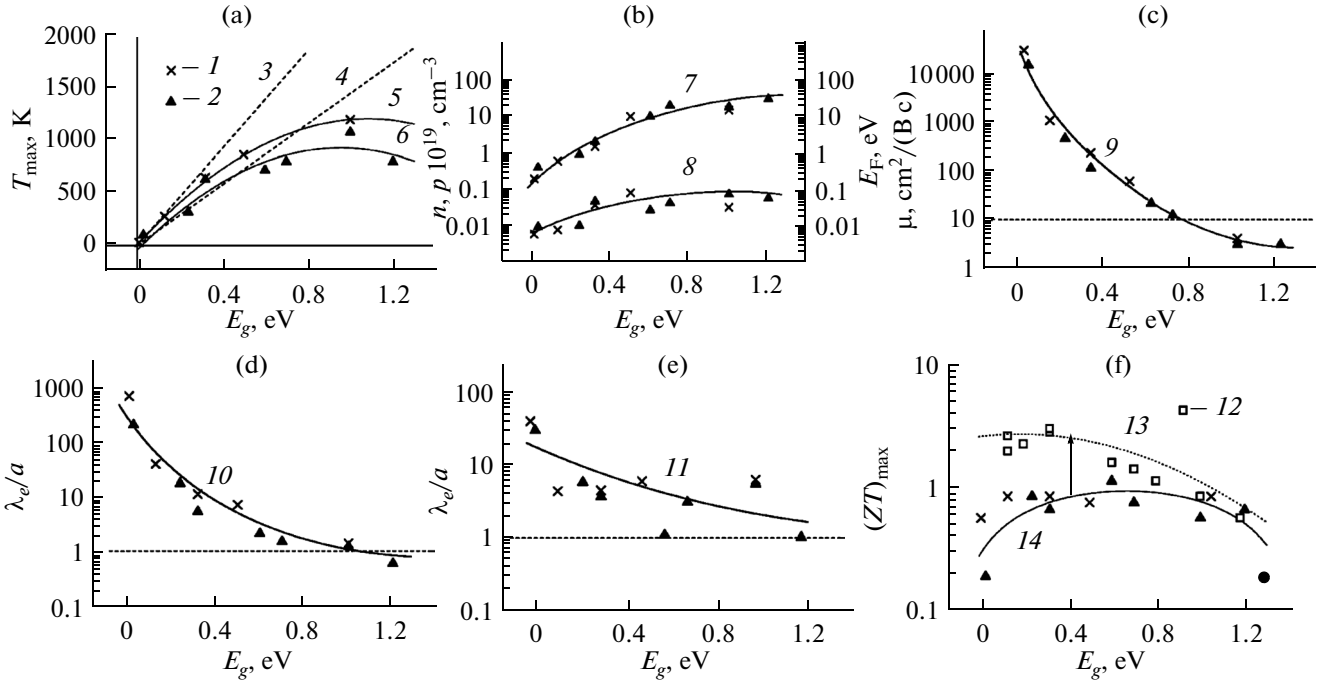

Fig. 3. The dependences of various parameters of TEM taken at the temperature $T = T_{max}$ on the bandgap E_g of samples (a–e): (a) T_{max} (*3–6*); (b) $n(p)$ (*7*) and E_F (*8*); (c) μ (*9*); (d) λ_e/a (*10*); (e) λ_{ph}/a (*11*); (f) $(ZT)_{max}$ (*12*, *13*, and *14*). (Samples: *3–11*, *14*—crystals; *12*, *13*—nanostructures. Data: *5–9*, *10*, *11*, *12*, *14*—experiment; *3*, *4*, *13*—calculation. Calculation formulas: *3*, *4*—$E_g = bk_0T$ (*3*—$b = 5$; *4*—$b = 10$; $k_0 = 1.38 \times 10^{-23}$ J/K is the Boltzmann constant); *13*—$y = (ZT_{max})$ (λ_{ph}/a). Materials (in increasing order of E_g): *n*-type: BiSb, Bi_2Te_3, PbTe, $CoSb_3$, and SiGe (points *1*); *p*-type: BiSb⟨Sn⟩, Sb_2Te_3, PbTe, TAGS, GeTe, SiGe, and $Cu_{1.99}Se$ (points *2*) [19, 21]).

The *ZT* dependences of TEM have peaks at the temperature T_{max} related to the development of intrinsic conductivity in the samples at the increase in temperature [12, 16, 17].

In Fig. 3, the dependences of various parameters of TEM on the value of the bandgap are shown. As a result of the analysis of the T_{max} dependence on the E_g value for materials of *n*- and *p*-type conductivities (see Fig. 3a, curves *5* and *6*), the optimal working temperatures, the electron *n* and hole *p* concentrations, and the Fermi energy E_F depending on the E_g value of the samples were determined (see Fig. 3b, curves *7* and *8*) [19]. A nonlinear character of the dependences $T_{max} = f(E_g)$ (see Fig. 3a, curves *5* and *6*) was explained by the decrease in the mobility μ of the samples for high E_g lower than the threshold value μ ~ 10 cm^2/(V s) (see Fig. 3c, curve *9*), which differentiates the materials with a band ($\lambda_e/a \gg 1$) and a jump conductivity ($\lambda_e/a = 1$) (see Fig. 3d, curve *10*), where λ_e is the average electron (hole) free track length in the samples and $a = 0.3$ nm is the shortest interatomic distance. The dependence of the average phonon free track length λ_{ph}/a on the value $E_g(T = T_{max})$ (see Fig. 3e, curve *11*) was also established, which made it possible to predict the increase in *ZT* of the samples at their nanostructuring through the formula $(ZT)_{NS} = (ZT)_{cryst}$ (λ_{ph}/a) (see Fig. 3e, curve *13*) [19, 20]. According to the evaluations (see Fig. 3f, curve *13*), nanostructuring can be efficient only for low-temperature TEM ($E_g << 0.8$ eV) (the increase in $(ZT)_{max}$ by ~3 times) (see Fig. 3f, arrow). For high-temperature TEM ($E_g > 0.8$ eV), nanostructuring proves significantly less efficient (see Fig. 3f, curve *13*), which is confirmed by the corresponding experimental data (points *12*) obtained by some researchers [17, 21].

The obtained curves (see Fig. 3) help to make a prediction of an unknown E_g value of TEM by a known T_{max} value (Table 1). In Table 1, the corresponding estimates of E_g for some TEM with high *ZT* values developed by researchers in recent years are shown [17]. In the evaluations of E_g for alloys with *n*- and *p*-type conductivities, curves *5* and *6* were used (see Fig. 3), and in the case of absence of accurate data on the type of conductivity of the samples, the corresponding dependences (curves *5* and *6*) were averaged. The signs (>) and (≥) given in Table 1 correspond to cases where the T_{max} range in the *ZT* temperature dependences was not reached at all or the researchers rather closely approached this range [17].

COMPUTER DESIGN OF WIDE-BANDGAP SEMICONDUCTORS WITH THE CHALCOPYRITE STRUCTURE

The information from the Bandgap DB was used to evaluate the bandgap of compounds with a chalcopy-

Table 1. Estimates of an unknown E_g value of TEM by a known temperature T_{max}

Class of material	Conductivity type and sample composition	$(ZT)_{max}$	T_{max}, K	Estimate of E_g, eV
Skutterudites	$p, n - Co_4Sb_{12}$	0.2	480	0.3
	$p, n - Yb_{0.19}Co_4Sb_{12}$	1.2	>680	>0.4
	$p, n - Ca_{0.18}Ni_{0.03}Co_{3.97}Sb_{12.4}$	1.0	>800	>0.55
	$p, n - Ba_{0.30}Ni_{0.05}Co_{3.95}Sb_{12}$	1.3	≥920	≥0.7
	$p, n - Ce_{0.9}Fe_3CoSb_{12}$	1.1	>760	>0.45
Clathrates	$n - Ba_8Ga_{16}Ge_{30}$	1.4	>800	>0.5
	$n - Ba_8Ga_{16}Si_{30}$	0.87	>900	>0.6
	$Ba_8Ga_{16}Ge_{30}$	0.7	≥800	≥0.5
Heusler phases	$p - TiNiSn$	0.45	650	0.45
	$n - Zr_{0.25}Hf_{0.25}Ti_{0.5}NiSn_{1-y}Sb_y$	1.4	700	0.4
	$n - Zr_{0.5}Hf_{0.5}Ni_{0.8}Pd_{0.2}Sn_{0.99}Sb_{0.01}$	0.7	800	0.45
	$Hf_{0.75}Zr_{0.25}NiSn_{0.975}Sb_{0.025}$	0.81	1025	1.0
Zintl phases	$p - Yb_{14}MnSb_{11}$	1.0	1200	1.0
Zn_4Sb_3 type	$p - Zn_4Sb_3$	1.3	670	0.5
Metal oxides	$p - NaCo_2O_4$	0.8	≥1000	≥1.1
	$p - Ca_3Co_4O_9$	1.0	>950	>0.9
	$n - (ZnO)_3(In_2O_3)\langle Ca\rangle$	0.31	>1053	>1.1
$FeSb_2$ type	$n - FeSb_2$	0.005	12	~0
Perovskites	$n - SrTiO_3\langle Nb\rangle$	0.37	1000	1.1
Thallium chalcogenides	$T_{l9}BiTe_6$	1.2	500	0.3
	Ag_9T1Te_5	1.23	>700	>0.4
	$p - T1In_{0.94}Yb_{0.06}Te_2$	1.8	700	0.5
Alkali metal chalcogenides	$p, n - CsBi_4Te_6$	0.8	225	0.15
	$n - K_2Bi_8Se_{13}$	0.2	300	0.2
	$p, n - K_2Bi_{8-x}Sb_xSe_{13}$	1.0	≥800	≥0.45
LAST-m	$p - AgPb_mSbTe_{m+2}$, $(m = 18–22)$	1.7	700	0.5
LASTT	$p - AgPb_mSn_nTe_{m+n+2}$	1.4	700	0.5
SOLT-m	$NaPb_mSb_nTe_{m+2}$ $(m = 20)$	1.6	675	0.5

rite crystal structure [22, 23], which was related to the search for new wide-bandgap semiconductors for optoelectronic devices [24]. Semiconductors are considered wide-bandgap if they have an interband electron transition energy that exceeds a value close to 2 eV [25].

The problem of the design of new chalcopyrites of the ABX_2 composition (A and B are various chemical elements; X is S, Se, Te, N, P, As, or Sb) with the bandgap higher than 2 eV under normal conditions was solved. To perform the calculations, the developed information-analytical system (IAS) for the computer design of inorganic compounds [23] including the databases on the properties of inorganic substances and a subsystem for the information analysis based on supervised pattern recognition was used. The procedure of such calculations is described in detail in [23, 26, 27].

The result of the computer analysis was a set of criteria having the form of various artificial intelligence formalisms (neural or growing pyramidal networks, logical expressions, etc.), which help to determine whether the compounds of the ABX_2 composition with the chalcopyrite structure refer to wide-bandgap semiconductors (i.e., they have $E_g > 2$ eV under normal conditions) or not [22, 23]. On the basis of the physicochemical presuppositions, the criteria included the following parameters of the elements A, B, and X:

—the function $\Delta\chi = |2\chi_X - \chi_A - \chi_B|$, where χ_i are the Martynov–Batsanov electronegativities;

Table 2. Comparison of the predictions of E_g with the experimental data for the studied chalcopyrites

Compound	E_{gexp}, eV	Prediction	Compound	E_{gexp}, eV	Prediction
$CuAlS_2$	3.5	>2 eV	$ZnGeAs_2$	1.16	<2 eV
$CuGaS_2$	2.44	>2 eV	$ZnSnP_2$	1.45	<2 eV
$CuInS_2$	1.5	<2 eV	$ZnSnAs_2$	0.74	<2 eV
$CuAlSe_2$	2.67	>2 eV	$ZnSnSb_2$	0.4	<2 eV
$CuGaSe_2$	1.63	<2 eV	$CdSiP_2$	2.2	>2 eV
$CuInSe_2$	0.95	<2 eV	$CdGeP_2$	1.8	<2 eV
$CuAlTe_2$	2.06	>2 eV	$CdGeAs_2$	0.53	<2 eV
$CuGaTe_2$	1.18	<2 eV	$CdSnP_2$	1.16	<2 eV
$CuInTe_2$	0.88	<2 eV	$CdSnAs_2$	0.3	<2 eV
$AgAlS_2$	3.13	>2 eV	$AgInS_2$	1.9	<2 eV
$AgGaS_2$	2.75	>2 eV	$CdSiAs_2$	1.51	<2 eV
$AgAlSe_2$	2.55	>2 eV	$CuFeS_2$	0.53	<2 eV
$AgGaSe_2$	1.65	<2 eV	$CuFeSe_2$	0.16	<2 eV
$AgInSe_2$	1.24	<2 eV	$CuFeTe_2$	0.1	<2 eV
$AgAlTe_2$	1.8	<2 eV	$LiGaTe_2$	2.31	>2 eV
$AgGaTe_2$	1.1	<2 eV	$LiInTe_2$	1.46	<2eV
$AgInTe_2$	0.96	<2 eV	$AgFeSe_2$	0.23	<2 eV
$ZnSiP_2$	2.07	>2 eV	$MgSiP_2$	2.35	>2 eV
$ZnSiAs_2$	2.1	>2 eV	$MnGeP_2$	0.24	<2 eV
$ZnGeN_2$	2.9	>2 eV	$MnGeAs_2$	0.6	<2 eV
$ZnGeP_2$	2.1	>2 eV			

—the valences Z_A, Z_B, and Z_X (for transition metals it is the group number);

—the average number of valence electrons: $n = (n_A + n_B + 2n_X)/4$;

—the electronegativities by the Pettifor scale [28]

—the function $(I_z/Z)_A - \{6 + 0.1(I_z/Z)_C\}$, where I_z is the last ionization potential.

In Table 2, the results of the use of the obtained criteria for the evaluation of the bandgap for chalcopyrites, whose data were used in the computer analysis of experimental data from the Bandgap DB, are shown.

Table 3. Predicted E_g for chalcopyrites whose data were not used in the computer analysis

Compound	Predicted E_g
$ZnAlS_2$	>2 eV
$ZnAlSe_2$	>2 eV
$ZnAlTe_2$	<2 eV
$AgFeS_2$	<2 eV
$AgFeTe_2$	<2 eV
$ZnGaTe_2$	<2 eV
$CdGaTe_2$	<2 eV
$HgGaTe_2$	<2 eV

The correspondence between the experimental and the predicted E_g values was observed (see Table 2), which proved the validity of the applied computer methods. Using the found criteria, E_g of chalcopyrites (Table 3) was evaluated, for which there was no corresponding information in the Bandgap DB. According to the predictions, $ZnAlS_2$ and $ZnAlSe_2$ chalcopyrites belong to wide-bandgap semiconductors, which makes them promising for optoelectronic applications.

CONCLUSIONS

1. A specialized database Bandgap on the bandgap containing more than 5500 records on about 3000 inorganic substances and materials was developed.

2. The Bandgap DB is available via the Internet (http://bg.imet-db.ru) and is integrated with other information systems on the properties of inorganic materials, which significantly widens its capabilities for the search of information on a specific substance.

3. The use of the Bandgap DB for the analysis of information on thermoelectric materials was demonstrated by citing specific examples.

4. The possibility of use of the information from the DB for the ab initio computer prediction of an

unknown E_g value was shown by the example of semiconductors with the chalcopyrite structure.

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