Advanced Physical Research
Vol.2, No.1, 2020, pp.26-36

CALCULATION OF ELECTRONIC STRUCTURE OF TRIPLE TYPE COMPOUNDS $A^{III}B^{III}X^{VI}_2$ WITH CHAIN STRUCTURE

E.M. Gojayev[*], **Z.A. Jahangirli**

Azerbaijan Technical University, Baku, Azerbaijan

Abstract. In the presented paper, based on first-principles calculations within the pseudopotential theory calculated the band states of crystals $A^{III}B^{III}X^{VI}_2$ with tetragonal lattice structure. According to the calculated band structure of the compound $TlInSe_2$, $TlGaTe_2$, $InGaSe_2$, $TlInTe_2$, $InGaTe_2$ valence band can be divided into three subgroups. The upper band width of ~ 4eV, owes its origin to p-states Tl_I, Tl_{II} and chalcogenides. Analysis of the wave functions of the valence states shows that the lowest group of about -12 eV, which consists of four zones must originate s-states of the cation. In the s-band spectrum of the state of chalcogenides and *s*-, *d*-state cations III groups form separate groups. Comparison of calculated results with the available theoretical and experimental data shows satisfactory agreement, including the band gap of the above compounds

Keywords: *Electronic structure, pseudopotential, band structure, form factors, chain structure, ternary chalcogenides.*

Corresponding Author: *E.M. Gojayev, Azerbaijan Technical University, Baku, AZ-1073, Azerbaijan, e-mail: geldar-04@aztu.edu.az*

Received: *27 February 2020;* ***Accepted:*** *24 May 2020;* ***Published:*** *30 June 2020.*

1. Introduction

It is known that the search for new semiconductor materials is usually carried out in the direction of expanding the crystal structure group of already known materials. Deciphering the crystal structure of TlSe revealed that this phase is distinguished by specific features. The TlSe lattice turns out to be composed of two independent structural units - an eight-vertex with the ionic nature of the Tl + –Se bond and a tetrahedron with a covalent bond between Tl_3 + -Se and, therefore, the chemical formula of TlSe should be written as Tl + Tl + $3Se_2$ (Mooser & Pearson, 1956). By replacing the trivalent thallium atom with the corresponding trivalent atoms, gallium and indium in the TlSe lattice, a new class of semiconductor compounds of the type are obtained. X-ray diffraction studies (Mooser & Pearson, 1956; Müller *et al.*, 1973; Hahn & Weltman, 1967) showed that some of these compounds have a chain, and the other part has a layered structure. Compounds with a chain structure crystallize in tetragonal syngony, space group (I4/mcm). According to studies of the crystal structure, properties and applications of the compounds $TlInSe_2$ (Te_2), $TlGaTe_2$, $InGaSe_2$ (Te_2), a lot of information is available in the domestic and foreign literature (Gojayev *et al.*, 2004; Godjaev *et al.*, 2007; Godzhaev *et al.*, 2009; Godjaev *et al.*, 2011; Hanias *et al.*, 1993; AlOrainy, 2012; Gojayev *et al.*, 2006; Mobarak *et al.*, 1997; Deiseroth *et al.*, 1985; Gojaev *et al.*, 2010; Nagat *et al.*, 2015; Abay *et al.*, 1996; Blachnik & Klose, 2000; Al-Ghamdi, 2004; Hussein, 1989; Rajesh & Philip, 2003; Karakotsov & Anagnostopoulos 1993; Abay *et al.*, 1996). However, the calculation of the energy spectrum using modern methods and programs, system analysis, and identification of the results of compounds of the type having a chain crystal structure were not carried out. In this work, we present the results of calculating the energy spectra of the compounds $TlInSe_2(Te_2)$, $TlGaTe_2$, $InGaSe_2(Te_2)$ crystallizing in the same tetragonal syngony. For calculations, the pseudopotential method was used.

This method is one of the main methods for calculating the energy spectrum of semiconductor charge carriers and is widely described in (Konstantinov *et al.*, 1977; Austin *et al.*, 1962; Bachelet *et al.*, 1982). The idea of the pseudopotential method was first encountered in the work of Philips (Phylipps, 1958). To calculate the band structure of diamond, Philips acted as follows: first, the effective electron potential is constructed near the Fermi level, which consists of two parts - the first is connected electrons, the second is connected with the core electrons. Then, the second part of the effective potential, which is associated with the core electrons, is replaced by the repulsive potential. In this case, it was possible to greatly reduce the number of plane waves taken into account in the expansion of the electron wave function. So, in the case it turned out to be sufficient to take 27 plane waves to obtain the results of the calculation of orthogonolized plane waves (OPW) of German (German, 1954). The arbitrary constants of the approximate potential were determined in two ways: by comparing with the electron spectrum calculated by the OPW method and by satisfying the experimental values of the direct and indirect energy gap. Both results are in good agreement with each other.

Later in (Phylipps & Kleinman, 1959), Phylips and Kleiman, developing the pseudopotential method, gave him a more rigorous formulation. Their method was based on the Herring OPV method, the essence of which is that the orthogonalization of plane waves to the wave functions of the inner shells leads to rapidly converging expansions for electronic wave functions.

2. Results and discussion

In all cases, the theory of pseudopotential is based on three fundamental physical approximations.

1. The first approximation is the self-consistent field approximation. In this approximation, the interaction between the electrons is described by a certain average potential, which itself depends on what states the electrons are in, the electronic states, in turn, are determined by the average potential.

2. In a second approximation, all electronic states are divided into inner shells (“core”) and states of the conduction band, and it is assumed that the wave functions of the inner shells are strongly localized.

3. The third fundamental approximation is the use of perturbation theory for electrons in the conduction band.

In [28], the pseudopotential method was substantiated from the point of view of scattering theory. The idea of the method is to replace the atomic potential inside the sphere with a radius R_M with a model potential that has exactly the same properties as the true potential with respect to the action on an external particle with energy E.

The eigenvalues of the energy E (k) for a certain quasi-wave vector k can be found by solving the Schrödinger equation in the representation of plane waves

$$\det\left|\left[\frac{1}{2}(\mathbf{k}-\mathbf{g})^2-E\right]\delta_{\mathbf{gg}'}+V\left(\mathbf{k}-\mathbf{g},\mathbf{k}-\mathbf{g}'\right)\right|=0,$$

Here **g** and **g'** are the reciprocal lattice vectors, and $V\left(\mathbf{k}-\mathbf{g},\mathbf{k}-\mathbf{g}'\right)$ is the matrix element of the pseudopotential $V_{ps}(\mathbf{r})$.

The full pseudopotential $V_{ps}(\mathbf{r})$ is the sum of the overlapping pseudopotentials of spherical atoms located at the points R_j.

$$V_{ps}\left(\mathbf{r},\mathbf{r}'\right)=\sum_j v\left(\mathbf{r}-\mathbf{R}_j,\mathbf{r}'-\mathbf{R}_j\right)$$

$V\left(\mathbf{r},\mathbf{r}'\right)$-full pseudopotential of the crystal; $v\left(\mathbf{r},\mathbf{r}',\mathbf{R}_j\right)$- atomic pseudopotential. Matrix elements $V_{ps}\left(\mathbf{r},\mathbf{r}'\right)$ calculated in a system of plane waves.

$$\left\langle\mathbf{k}-\mathbf{g}\middle|V\left(\mathbf{r},\mathbf{r}'\right)\middle|\mathbf{k}-\mathbf{g}'\right\rangle$$

Let us denote $\mathbf{K}=\mathbf{k}-\mathbf{g}$, $\mathbf{K}'=\mathbf{k}-\mathbf{g}'$, $\mathbf{G}=\mathbf{K}-\mathbf{K}'$ then, $\left\langle\mathbf{K}\middle|V\middle|\mathbf{K}'\right\rangle=S(\mathbf{G})v(\mathbf{K},\mathbf{K}')$ here $S(\mathbf{G})=\frac{1}{N}\sum_j\exp\left(-i\mathbf{G}\mathbf{R}_{\mathrm{j}}\right)$ the structural factor $v\left(\mathbf{K},\mathbf{K}'\right)$ is the form factor.

$$v\left(\mathbf{K},\mathbf{K}'\right)=\frac{1}{\Omega}\int\exp\left(-i\mathbf{K}\mathbf{r}\right)v\left(\mathbf{r},\mathbf{r}'\right)\exp\left(i\mathbf{K}'\mathbf{r}\right)d\mathbf{r}d\mathbf{r}',$$

here N is the number of atoms in the system, Ω is the volume per atom. If a crystal consists of several elements, then α

$$\left\langle\mathbf{K}\middle|V\middle|\mathbf{K}'\right\rangle=\sum_\alpha S_\alpha(\mathbf{G})V_{\alpha c}\left(\mathbf{K},\mathbf{K}'\right)$$

$$S_\alpha(\mathbf{G})=\frac{1}{N_{\alpha c}}\sum_{cell}\exp\left(-i\mathbf{G}\mathbf{R}_{j\alpha}\right)$$

$$v_a\left(\mathbf{K},\mathbf{K}'\right)=\frac{1}{\Omega}\int\exp\left(-i\mathbf{K}\mathbf{r}\right)v_a\left(\mathbf{r},\mathbf{r}'\right)\exp\left(i\mathbf{K}'\mathbf{r}\right)d\mathbf{r}d\mathbf{r}'$$

Ω_c - is the unit cell volume; $N_{\alpha c}$ - is the number of atoms type α.

In the approximation of the Hubbard-Shem model using the dielectric function, we can write

$$v\left(\mathbf{K},\mathbf{K}'\right)=\frac{v^{ion}\left(\mathbf{K},\mathbf{K}'\right)}{\varepsilon(\mathbf{G})},$$

where:

$$\varepsilon(\mathbf{G})=1-\frac{8\pi e^2}{\Omega\mathbf{G}^2}\left[1-\frac{\frac{1}{2}\mathbf{G}^2}{\mathbf{G}^2+k_F^2+k_S^2}\right]\chi(\mathbf{G}),$$

$$\chi(\mathbf{G})=-\frac{1}{2}z\left(\frac{2}{3}E_F\right)^{-1}\left(\frac{1}{2}+\frac{4k_F^2-\mathbf{G}^2}{8\mathbf{G}k_F}\ln\left|\frac{2k_F+\mathbf{G}}{2k_F-\mathbf{G}}\right|\right)$$

z-is the number of valence electrons per atom, E_F - is the Fermi energy, k_F - is the Fermi wave vector, k_S - is the screening parameter

$$k_F = \sqrt{3\pi^2 n}\,,\ E_F = \frac{k_F^2}{2}\,,\ k_S = \sqrt{\frac{2k_F}{\pi}}\,.$$

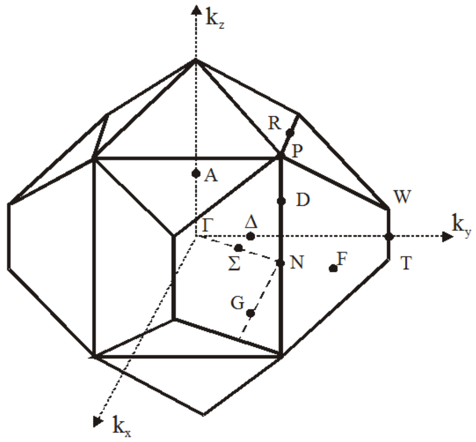

Fig. 1. Brillouin zone of the base-centered lattice $TlGaTe_2$

The band structure $TlGaTe_2$ was first calculated in (Okazaki *et al.*, 2001) by the empirical pseudopotential method. The form factors of atomic pseudopotentials were calculated using the analytical expression proposed in (Okazaki *et al.*, 2001). The calculations showed that the ceiling of the valence band is located at the highly symmetric point T (0, 2π/*a*, 0) on the boundary of the Brillion zone (BZ), and the bottom of the conduction band on the line D (π/*a*, π/*a*, k) also the boundary of the BZ volume-centered tetragonal (VCT) lattice. The authors concluded that a direct transition is forbidden for the compounds $TlGaTe_2$ according to the selection rules. The character tables of the irreducible and double-valued irreducible representations of the groups of wave vectors of the I4/mcm spatial group were obtained in (Gashimzadeh, 1960). The compatibility conditions for irreducible representations of simple groups and two-valued groups D_{4h}^{18} are given here. The form of the BZ (Fig. 1) for a body-centered tetragonal lattice (c with the axis ratio $c/a < 1$) is also given in this work.

The calculation of the band structure of the compound $TlGaTe_2$ was also carried out using the (German, 1954; Gashimzade & Orujov, 1980) pseudopotential method.

The lattice parameters a = 8.429(6) Å, c = 6.865(4) Å and the chalcogen parameter $x = 0.170$ were taken from (Müller *et al.*, 1973).

From fig. 2, where the zone structure of the $TlGaTe_2$ is presented, the following main conclusions can be drawn:

1. The valence band ceiling is located at the highly symmetric point T on the surface BZ and corresponds to the irreducible representation of T_3, and the bottom of the conduction band on line D is in the middle between points $P(\pi/a, \pi/a, \pi/c)$ и $N(\pi/a, \pi/a, 0)$, corresponds to the irreducible representation D1. The least direct transition in energy occurs between the states T_3 and T_4, which is forbidden in the dipole approximation. The band gap obtained from the calculations is 0.86 eV.

2. Valence zones can conditionally be divided into three groups. The lowest, consisting of 4 zones, a group of about -11 eV, owes its origin to 5s states. Another group of 4 zones in the region of -4: -6 eV mainly comes from 6s states of atoms and 4s

states of atoms. The upper group of ten bands in the region of 0 -4 eV is mainly composed of 5p atomic states, 6p atomic states and 4p atomic states. In addition, we found that 6s states of atoms take part in the formation of bands in the vicinity of the top of the valence band T_3.

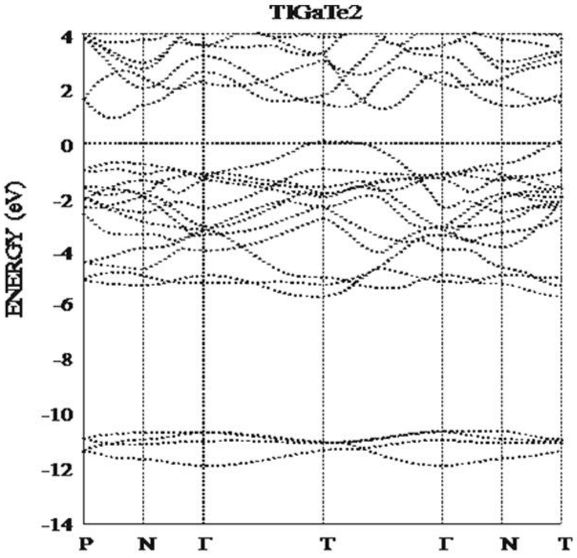

Fig. 2. The Band structure of $TlGaTe_2$

These results on the origin of the bands are consistent with the data of (Okazaki *et al.*, 2001), where the photoemission spectra were studied, and the band structure $TlGaTe_2$ was calculated by the method of coupled plane waves. But in this band picture, the valence band overlaps with the conduction band, which contradicts the experimental facts.

The electronic spectrum of the $InGaTe_2$ compound was calculated using the density functional method using the ABINIT software package. In the expansion of the wave function, plane waves with a maximum kinetic energy were used 60 Ry. The lattice parameters were determined by minimizing the total energy, and the structure parameters were optimized using the Gelman-Feynman forces. The process of minimizing the forces was carried out until the force moduli satisfied the condition $\left|\vec{F}\right|$ <3 $\frac{mRy}{a.u.}$. To calculate the band structure of $InGaTe_2$, the optimized lattice parameters are a = 8.3945 Å c = 6.8352 Å, and chalcogen parameter x = 0.1730.

The electronic spectrum $InGaTe_2$ was calculated at the symmetric points Γ, T, N, P, as well as along the lines connecting these points. The results of the calculation of the band structure are shown in Fig. 3.

As can be seen from the figure, the valence band consists of three subbands. The lower subband, consisting of four zones, is distant from the others by a wide energy gap of the order of ~ 6 eV. Group theoretical analysis shows that these lower valence bands located near -10 -11 eV are due to the 5s states of Te. The next group of four valence bands located at an energy level of about -5 eV comes mainly from the s-states of In and Ga atoms. The remaining large group of ten bands with a width of 5 eV comes from the p states of In, Ga, and Te atoms. In (Mobarak *et al.*, 1997), where the X-ray photoemission spectrum is shown, it was revealed that the photoemission spectrum consists of three distinct regions. These authors attribute the peak at −11.5 eV to the 5s – states of Te, the peak near –4 eV to Ga – Te bonds, and the complex of features near –5 0 eV to Ga – Ga and Ga – Te bonds, which is in good agreement with our calculation of the band spectrum and group-theoretical analysis. The band gap from our calculations is 0.56 eV.

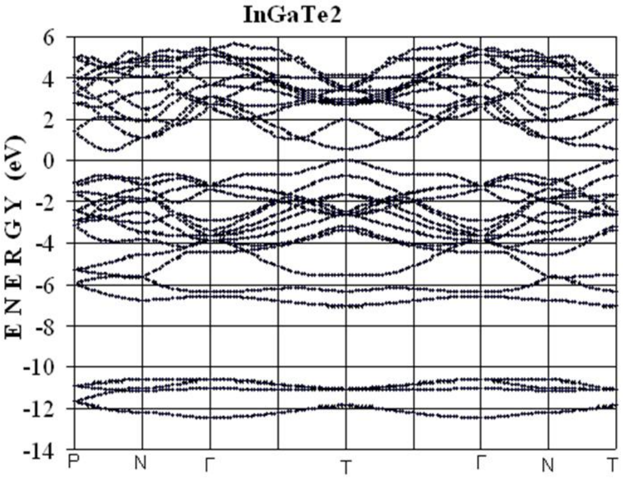

Fig. 3. The Band structure of $InGaTe_2$

In this work, the band spectrum was also studied, and was determined the genesis of the electronic states of the crystal $InGaTe_2$. The calculation of the electronic structure was carried out in the framework of the theory of the functional of local electron density by the pseudopotential method in the basis of plane waves.

The semiconductor compound $InGaTe_2$ belongs to the tetragonal group D_{4h}^{18}, the unit cell contains two formula units, lattice constants a = 8.0511 Å, c = 6.3174 Å, and chalcogen parameters x = 0.1636 (Müller *et al.*, 1973). In the crystal lattice $InGaTe_2$, monovalent In atoms are surrounded by eight Te atoms, while threevalent Ga atoms are in the tetrahedral environment of Te atoms and form atomic chains $(Ga_3^+ Se_2^{-2})$ - extended along the optical axis $\vec{c}$.

The lattice parameters were determined by minimizing the total energy, and the structure parameters were optimized using the Gelman-Feynman forces. The process of minimizing the forces was carried out until the force moduli satisfied the condition $\left|\vec{F}\right|$ $<3\ \frac{mRy}{a.u.}$. Optimized lattice parameter a = 8.0138 Å, c = 6.9534 Å, chalcogen parameters x = 0.1720.

The band spectrum $InGaSe_2$ is shown in Fig. 4. The ceiling of the valence band is selected for zero energy. The main feature of the valence band is that it consists of pronounced three subbands separated by forbidden energy regions. The lowest subband, consisting of four zones, lies apart, about -10÷-11eV and is distant from the others by a_0 wide energy gap of the order of ~ 6 eV. The results of group-theoretical analysis using crystal symmetry properties $InGaSe_2$ show that these valence bands are due to the 5s states of Se. The next group, located at an energy level near -5 eV, consists of four valence bands formed from the 5s states of In atoms and 4s states of Ga atoms. The uppermost subband, consisting of ten bands ~ 5 eV wide, occurs mainly from the p states of In, Ga, and Se atoms.

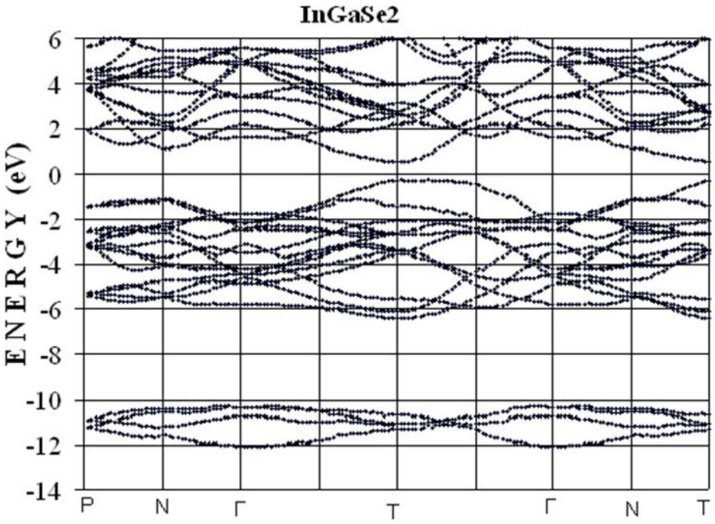

Fig. 4. The Band structure of $InGaSe_2$

Using the pseudopotential method, the band structure of the compound $TlInTe_2$ was calculated taking into account the nonlocality of pseudopotentials. Crystal lattice parameters: a = 8.494 Å, c = 7.181 Å and the chalcogen parameter x = 0.1813 used in the calculations was taken from (Müller *et al.*, 1973). The calculation results are shown in Fig. 5.

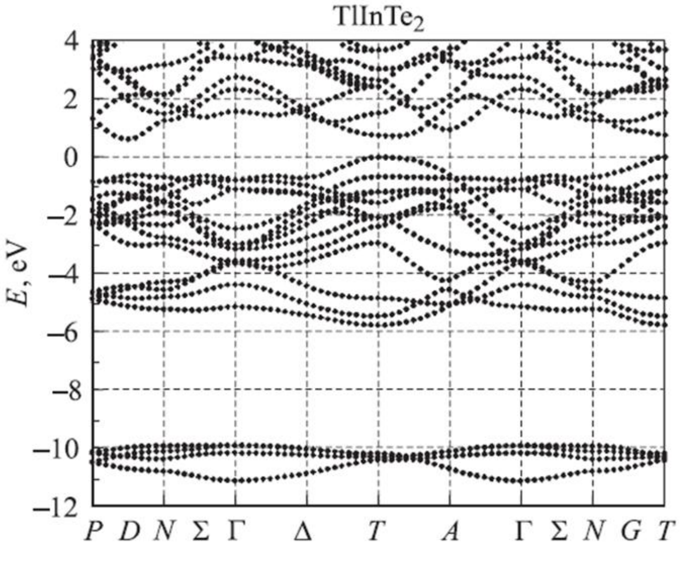

Fig. 5. The Band structure of $TlInTe_2$

An analysis of the obtained results shows that the ceiling of the valence band is located at the highly symmetric point $T(0.2\pi/a.,0)$ on the surface of the BZ and corresponds to the irreducible representation of T_3, and the bottom of the conduction band on line D $(\pi/a,\pi/a,k)$, also located on the surface of the BZ in the middle between points $P(\pi/a,\pi/a,\pi/c)$ and $N(\pi/a,\pi/a,k,0)$, corresponds to the irreducible representation of D_1. The band gap 0.66 eV obtained from the calculations is in good agreement with experimental data (Orudzhev *et al.*, 2003). The lowest energy direct transition occurs approximately at point T between the states T_3 and T_4. According to the selection rules, the transition T_3 and T_4 is forbidden in the dipole approximation. The bottom of the conduction band at point T (state T_4) is a saddle point. The minimum is located near the point T(0,0, $2\pi/c$), which is the equivalent of T outside the BZ, namely, at a point $A\left[0,0,(\pi/c)\left[1+(c/a)^2\right]\right]$ on the border of the BZ along the line A (the highest point of the BZ in Fig. 5.) and corresponds to the irreducible representation A_2.

The third largest minimum of the conduction band is also located on line A at point A(0,0,π/c) and corresponds to the irreducible representation of A_4.

Valence zones in composition and nature can be divided into three groups. According to the group-theoretical analysis that we used using the symmetry properties of TlSe crystals (Gashimzadeh, 1960), the lowest four-band group, about -11 eV, owes its origin to 5s Te states. The middle group of four bands in the range from -3.5 eV to -6 eV mainly comes from 6s states of Tl atoms and 5s states. The upper group, the most complex in structure, consisting of ten overlapping zones in the region from 0 to -3.5 eV, is mainly composed of 5p states of Te atoms, 6p states of Tl atoms and 5p states of atoms In. It should be noted that in the vicinity of the top of the valence band, the states of a monovalent ion Tl^+ also begin to appear, the main contribution of which is observed at point T. In the formation of the two lower conduction bands, the main contribution is made by the threevalent ion In^{3+} participating in the formation of ion-covalent bonds with ions Te^{2-}.

Using the pseudopotential method was calculated the energy spectrum of $TlInSe_2$. It was revealed that the ceiling of the valence band is located at a highly symmetric point T on the surface of the BZ and corresponds to the irreducible representation T_3, and the bottom of the conduction band is located on the line D in the middle between the points $P(\pi/a,\pi/a,\pi/c)$ and $N(\pi/a,\pi/a,0)$, that corresponds to the irreducible representation of D_1 (Fig. 6).

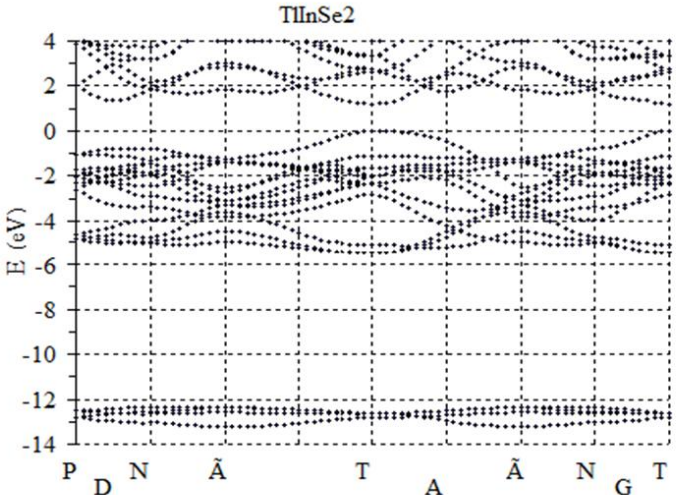

Fig. 6. The band structure of $TlInSe_2$

The least energy transition is occurs between the states T_3 and T_4 and forbidden in the dipole approximation. The band gap obtained on the basis of calculations is about 1 eV. The valence band can be divided into three groups. The lowest, with four bands at about -12.6 eV, owes its origin to 4s states Se. Another group of four bands in the region - (4-5.5) eV, is mainly due to the 6s states of atoms and 5s states. The upper group of ten bands in the region of 0-3.5 eV is mainly formed from the 4p state of Se atoms, the 6p state of atoms Tl and the 5p state of In atoms. The data on the origin of the bands are consistent with the results of (Gashimzade & Orujov, 1980), where the photoemission spectra were studied, and the band structure of $TlInSe_2$ was calculated by the method of plane-wave addition. However, in this band pattern, the valence band overlaps with the conduction band, which contradicts the experimental facts.

The theoretical conclusion of (Gashimzade & Orujov, 1980), which indicates that in the upper part of the valence band of the semiconductor compound $TlInSe_2$, there is an isolated group of two bands, is not confirmed in this work and in (Orudzhev *et al.*, 2003). This is probably due to the incorrect consideration of the screening of the pseudopotential inherent in the empirical method. In the same work, the imaginary and material parts of the complex permittivity, the optical absorption and reflection coefficients, as well as the effective number of valence electrons with polarization of the parallel and perpendicular optical axis are calculated. The result of these calculations is not in satisfactory agreement with the existing experimental data on $TlInSe_2$.

However, it was revealed for the first time (Orudzhev *et al.*, 2003) that the top of the valence band at point T originates mainly from the 6s states of thallium atoms. The authors of the same work found that in crystals of the type $TlSe \rightarrow Tl^{+}Tl^{3+}Se_2$, including in $TlInSe_2$, monovalent thallium atoms located in the eight-hole, providing the formation of lattices of the above type, simultaneously participate by $s-$electrons in the formation of the ceiling of their valence band and indirectly participate in the formation of physical properties these phases.

4. Conclusion

In the present work, based on calculations from first principles in the framework of the theory of pseudopotential, the band states of crystals of the type $A^{III}B^{III}X^{VI}_2$ are calculated. According to the calculated band structures of the compounds $TlInSe_2$, $TlGaTe_2$, $InGaSe_2$, $TlInTe_2$, $InGaTe_2$, the valence band can be divided into three subgroups. The upper group, ~ 4 eV wide, owes its origin to the p-states of TlI, TlII, and chalcogenides. Analysis of the wave functions of valence states shows that the lowest group, about -12 eV, consisting of four bands, owes its origin to the s-states of the cation. Separate groups form in the band spectrum of the s-state of chalcogenides and the s-, d-states of group III cations. A comparison of the calculated results with the available theoretical and experimental data shows a satisfactory correspondence of the band gap of the above compounds.

References

Abay, B., Gurbulak, B., Yildirim, M., Efeoglu, H., Tuzemen, S., Yogurtcu, Y.K. (1996). Electrothermal investigation of the switching effect in p-type $TlInSe_2$, $TlInTe_2$ and $TlGaTe_2$ chain chalcogenide semiconductors. *J. Electronic Mat*., 25, 1054-1059.

Al-Ghamdi, A.A., Hussein, S.A., Nassary, M.M. (2004). Memory switching effect in GaSe single crystals. *Mat. Sci. Res. India*, 2, 107.

AlOrainy, R.H. (2012). Interpretation of Switching Properties of $InGaSe_2$ Single Crystal. *Acta Physica Polonica A*, *121*(3), 666-672.

Austin, B., Heine, V., Sham, L.J. (1962). General theory of pseudopotentials. *Phys. Rev.*, *127*(7), 276-282.

Bachelet, G.B., Hamann, D.R., Schluter, M. (1982). Pseudopotentials that work: From H to Pu. *Phys. Rev. B*, *26*(8), 4199-4223.

Blachnik, R., Klose, E. (2000). Experimental investigation and thermodynamic calculation of excess enthalpies in Ga-In-Te system. *J. Alloy. and Comp*., 305, 144.

Deiseroth, H.J., Mueller, D., Hahn, H.Z. (1985). Strukturuntersuchungen an $InGaSe_2$ und $InGaTe_2$. *Anorg. Allg. Chem.*, 525, 163-172.

Gashimzade, F.M., Orujov, G.S. (1980). Calculation of the energy spectrum of electrons of ternary semiconductor compounds with the structure of thallium selenide, *Report of the Academy of Sciences of Azerbaijan*, *36*(12), 18-23.

Gashimzadeh, F. (1960). Symmetry of energy bands in type crystals, *FTT*, *2*(12), 3040-3044.

German, F. (1954). Calculation of the energy band structures of the diamond and germanium crystals by the method of orthogonalized plane waves. *Phys. Rev.*, *93*(6), 1214-1225.

Gojaev, E.M., Allakhyarov, E.A., Mamedov, E.M., Osmanova, S.S. (2010). X-ray diffraction characterization and electrical properties of $TlIn_{1-x}Ga_xTe_2$ crystals, *Inorg. Mater*., 46, 718.

Gojayev, E.M., Allakhyarov, E.A., Sadikhova, H.O. (1994) Tensometric properties of monocrystals $TlInTe_2$, *Inorganic materials*, *30*(6), 859

Godzhaev, E.M., Jafarova, S.R., Gulmamedov, K.D., Mammadov, E.M., Osmanova, S.S. (2009). Synthesis of growing single crystals of $TlInSe_2$ and $TlGaSe_2$. *Inorganic Materials*, *45*(7), 790-792.

Godjaev, E.M., Gulmamedov, K.D., Halilova, H.S., Gulieva, S.O. (2011). The switching effect on $TlInSe_2$ thin films. *Electronic Material Processing*, *47*(5), 18-22.

Gojaev, E.M., Gyulmamedov, K.D., Ibrogimova, A.R., Mousumov, A.A. (2010). Conductivity Piezomodulation in $InGaTe_2$ Single Crystals. *Inorg. Mater.*, 46, 353.

Gojayev, E.M., Kafarova, D.M. (2004) Thermal expansion and isothermal compressibility of $TlGaTe_2$. *Inorganic Materials*, *40*(9), 1060-1061.

Godjaev, E.M., Nazarov, A.M., Allakhyarov, E.A., Gulmamedov, K.D., Halilova, H.S., Mamedov, E.M. (2007). Acoustic-photovoltaic effect in $TlInSe_2$, $TlInTe_2$, and $TlGaTe_2$ single crystals. *Inorganic Materials*, *43*(10), 184-1189.

Gojayev, E.M., Orujov, G.S., Kerimova, R.A., Allahyarov, E.A. (2006). Band Structure and Optical Properties of a Chain Compound $TlInTe_2$. *Solid State Physics*, *48*(1), 40-43.

Hahn, H., Weltman, B. (1967). Üder ternare chalkogenide des Thalliums mit Gallium und Indium. *Naturwissenschaften*, *54*(2), 42.

Hanias, M., Anagnostopoulos, A.N. (1993). Negative-Differential-Resistance Effects in the $TlGaTe_2$ Ternary Semiconductor. *Physical Review B*, *160*(8), 4261-4266.

Hussein, S.A. (1989). Memory switching effect in single crystals of Thallium selenide. *Cryst. Res. Technol.*, 24, 467-474.

Karakotsov, Ch., Anagnostopoulos, A.N. (1993). Crisis in electrical behaviour of the $TlInSe_2$ semiconductor compound, *Physica B*, 93, 157-161.

Konstantinov, O.V., Nasibullaev, Sh.K., Panakhov, M.M. (1977). On the analytical expression for the pseudopotential form factors. *FTP*, *11*(5), 881-885.

Mobarak, M., Berger, H., Lorusso, G.F., Capozzi, V., Perna, G., Ibrahim, M.M., Margaritondo, G. (1997). The growth and characterization of $GaInSe_2$ single crystals. *J. Phys. D: Appl. Phys.*, 30, 2509-2516.

Mooser, E., Pearson, W.B. (1956). The chemical bond in semiconductors. *J. Electronics, 1*(6), 629-645.

Müller, D., Eulenberger, G., & Hahn, H. (1973). Über ternäre Thalliumchalkogenide mit Thalliumselenidstruktur. *Zeitschrift für anorganische und allgemeine Chemie*, *398*(2), 207-220.

Nagat, A.T., Abdulwahed, J.A.M., Alharbi, S.R., Saed, E.M., El-Saeedy, H.I. (2015). Negative-differential resistance effect in ternary chalcogenide semiconductor $InGaTe_2$, *International Journal of Scientific & Engineering Research*, *6*(1), 1233.

Okazaki, K., Tanaka, K., Matsuno, J., Fujimori, A., Mattheiss, L.F., Iida, S., Kerimova, E., Mamedov, N. (2001). Angle –resolved photoemission and band –structure results for linear chain $TlGaTe_2$. *Phys. Rev. B*, 64, 045210.

Orudzhev, G., Mamedov, N., Uchiki, H, Yamamoto, N., Iida, S., Toyota, H., Gojaev, E., Hashimzade, F. (2003). Band structure and optical functions of ternary chain $TlInSe_2$. *J. of Physics and Chemistry of Solids*, 64, 1703-1706.

Rajesh, R., Philip, J. (2003). Memory switching in In-Te glasses results of heat-transport measurements, *Semicond. Sci. Technol*., 18, 133-138.

Phylipps, J.C. (1958). Energy-band interpolation scheme based on a pseudopotential, *Phys. Rev.*, *112*(3), 685-695.

Phylipps, J.C., Kleinman, L. (1959). New method for calculating wave function in crystals and molecules. *Phys. Rev.*, *116*(2), 287-294.