



## Study of structural and electronic properties of AgCl and AgBr binaries

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### Abstract

This modest work was devoted to studying the structural and electronic properties of the AgCl and AgBr binaries in the cubic NaCl phase. In this study, we used the FP-LAPW method based on functional density theory (DFT). For the treatment of exchange potential and correlation, we used the local density approximation (LDA). The objective of this work is to predict and compare the structural and electronic properties of our materials with other theoretical and experimental results. Most of the results obtained were approximate.

**Keywords:** Structural and electronic properties, FP-LAPW, DFT, LDA.

### 1. Introduction

Silver halides have generated a lot of interest recently because of their importance as superionic conductors and being used as the main components in photographic materials. Thus, a good understanding of the physicochemical properties that occur in these fear systems requires a thorough knowledge of the structure of these compounds. The objective of this work is to predict and compare the structural and electronic properties of our materials. In this study, we used the FP-LAPW [1] method based on functional density theory (DFT) [2]. For the treatment of exchange potential and correlation, we used the local density approximation (LDA) [3]. Most of the results obtained in this work agree with other theoretical and experimental results.

### 2. General information on binary semiconductors I-VII

#### 2.1. Definition of semiconductors

The family of semiconductors is extensive since it ranges from the elements of a column (column IV) of the periodic table; Si and Ge to the compounds of several columns such as binary, ternary and quaternary. In this brief, we focus on I-VII binary semiconductors, especially the two AgCl and AgBr.

#### 2.2 Definition of binary semiconductor materials I-VII

Binary semiconductors I-VII are composed of an atom of column IB and another of column VIIB whose sum of valence electrons of the two atoms equals eight (8).

### 2.3 Physical properties of binary semiconductors I-VII

#### 2.3.1. Structural properties; crystalline structure [4]

Semiconductors come in several chemical compositions with a wide variety of crystalline structures. Binary compounds I-VII generally have three crystalline structures:

- Cubic centered faces (the NaCl structure (B<sub>1</sub>));
- Cubic centered (the CsCl structure (B<sub>2</sub>));
- The zinc blende structure (B<sub>3</sub>).

### 3. Calculation method

The structural and electronic properties of AgCl and AgBr binaries are calculated using the density functional theory (DFT) [2] all of which are computed using the total potential linear augmented plane wave (FP-LAPW) [1] method implemented in the Wien2k package [5]. Using LDA (Local Density Approximation), we investigated the effects of the exchange and correlation potential terms [3].

### 4. Results and discussion

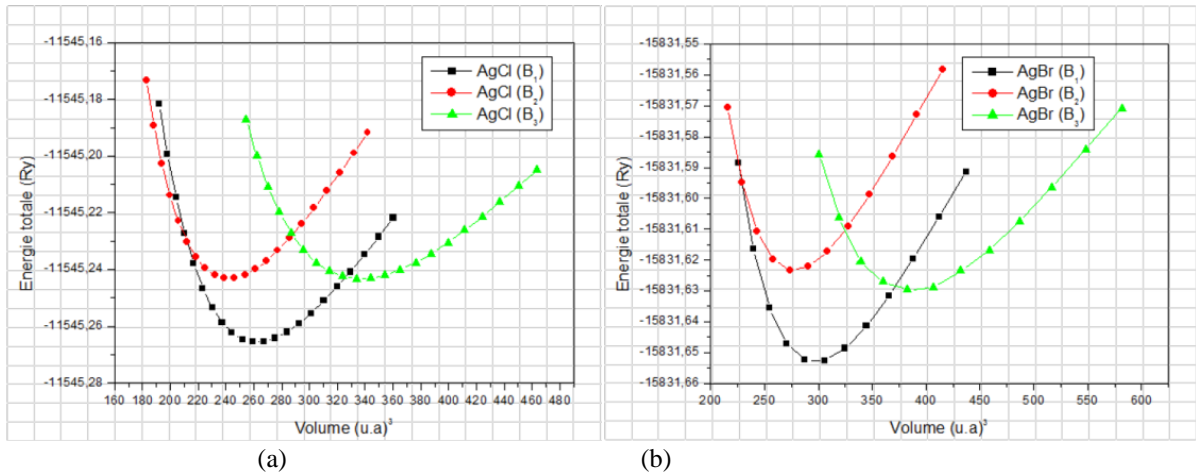
#### 4.1. Structural properties

This first part is the most important step in the development of the calculations, as the other properties depend on the optimized crystalline parameter. It consists in determining the grid parameter at equilibrium  $a_0$ , the compressibility module  $B_0$  and its derivative  $B'_0$ .

To determine the equilibrium structural properties of binary AgCl and AgBr, we calculated the total energy for several parameters of the "a" network in the vicinity of the  $a_{exp}$  experimental parameter, then we interpolated these values using the Birch state equation [6] given by:

$$E(V) = E_0 + \frac{9}{8} B_0 V_0 \left[ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^2 + \frac{9}{16} B_0 V_0 (B' - 4) \left[ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^3$$

Figure (1) represents the change in total energy as a function of unit volume in the three structures for binary AgCl and AgBr, respectively.



**Figure 1.** Optimization of total energy as a function of volume using the LDA approximation: (a) AgCl; (b) AgBr.

From figure 1(a,b) it can be deduced that the lowest minimum of the energy curves of the two binaries in the three phases  $B_1$ ,  $B_2$ , and  $B_3$  is that of the curve corresponding to the structure  $B_1$  which is the most stable structure. So we can say that both the binary AgCl and AgBr crystallize under the NaCl structure ( $B_1$ ).

Table (1) shows the structural results obtained for binary AgCl and AgBr in comparison with those obtained by experience and by the theoretical calculation of other researchers using other methods.

**Table 1.** Calculated lattice parameter ( $a_0$ ), bulk modulus ( $B_0$ ) and its pressure derivatives ( $B_0'$ ) for AgCl and AgBr.

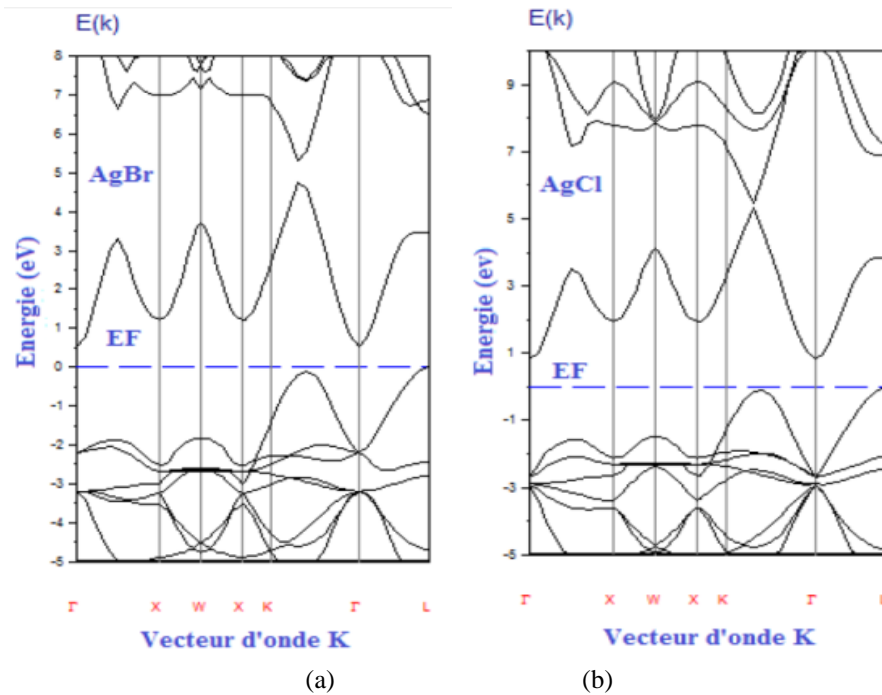
	$a_0$ (Å)	$B_0$ (GPa)	$B_0'$
AgCl	5.38	68.37	5.23
	5.39	66.8	5.2
	[7]	[8]	[8]
AgBr	5.6	62.20	5.3
	5.58	60.3	5.1
	[7]	[8]	[8]

The values obtained from cell parameters  $a_0$  and  $B_0'$  for the AgCl and AgBr binaries are in good agreement with some theoretical results [7] and close to the experimental results [9]. However, the  $B_0$  values obtained are higher than the experimental values [9].

### 5.2. Electronic properties

The band structure calculations for the two binary compounds AgCl and AgBr were performed using the equilibrium network parameter.

The band structures for the two calculated binaries at the equilibrium mesh parameters are shown in Figure 2.



**Figure 2.** Band structure along the symmetry lines of the Brillouin zone at the equilibrium lattice constant for AgCl and AgBr in the (B<sub>1</sub>) phase. The position of the Fermi level is shown by the horizontal line: (a) AgBr; (b) AgCl.

From these figures, we can see the indirect gap semiconductor behavior of these compounds. The maximum of the valence band is located at point L for both binaries but the minimum of the conduction band is located at point  $\Gamma$ .

The calculated bandwidth energies of the two binaries in phase B<sub>1</sub> in comparison with those obtained by experiment and theoretical calculations are summarised in the table (2).

**Table 2.** Gap energies in (eV) AgCl and AgBr binaries in phase B<sub>1</sub>.

	AgCl	AgBr
$E_{g(\Gamma-L)}(eV)$	0.830336	0.53129
	0.95 [10]	0.71 [10]

It should be noted that the gap values calculated by LDA are lower than the experiment values and not far from the few theoretical results obtained by the same exchange-correlation approximation. This underestimation of the gap values is mainly due to the fact that the LDA does not take into account the energy independence of quasi-particles correctly [11].

## 5. Conclusion

The purpose of this paper was to present a theoretical study on the structural and electronic properties of AgCl,

and AgBr semiconductor materials using the FP-LAPW method. In this method, the potential user is based on the local density approximation (LDA) for the calculation of the exchange and correlation energy used in the density functional theory (DFT).

For the structural properties, we identified the structure in which the two AgCl and AgBr binaries crystallized among the structures (B<sub>1</sub>, B<sub>2</sub>, B<sub>3</sub>), and found that the structure (B<sub>1</sub>) NaCl is the appropriate structure. We also identified the properties of the static equilibrium, which tells that the parameters of the a<sub>0</sub> network, the compressibility module B<sub>0</sub>, and its derivative B<sub>0</sub>' in phase B<sub>1</sub> for both binaries (AgCl, AgBr)

Regarding the electronic properties, we calculated the band structure for each material in the B<sub>1</sub> structure, the results showed that each one has an indirect gap.

Knowing that the results we obtained were in good agreement with other theoretical and experimental results. This proves the accuracy of the method used (FP-LAPW).

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