



# Structural, elastic, thermal, electronic and optical properties of Ag<sub>2</sub>O under pressure



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## ABSTRACT

In present paper, the structural, elastic, thermal, electronic, optical properties at ambient and high-pressure study of Ag<sub>2</sub>O are performed using the full-potential linearized augmented plane wave (FP-LAPW) method within the framework of Density functional theory (DFT) as implemented in Wien2k Code. We have used the local density approximation (LDA), Generalized Gradient approximation (GGA) and Engel–Vosko generalized gradient approximation (EV–GGA) for calculating structural properties at 0.0–20.0 GPa pressure. The lattice constant obtained at 0.0 GPa using GGA method, is in good agreement with available experimental results. Decrease in lattice constant is observed with increase in pressure from 0.0 to 20.0 GPa. The electronic, optical and band structure calculations are also carried out using modified Becke–Johnson exchange correlation potential plus generalized gradient approximation (mBJ–GGA). At zero pressure, the calculated band gap using mBJ potential is found to be narrow, direct and comparatively better than calculated through LDA, GGA and EV–GGA. Also, the band gap increases with increase in pressure from 0.0 to 20.0 GPa. From elastic calculations, it is noted that Ag<sub>2</sub>O is elastically stable and have ductile nature. Moreover, it is revealed that Ag<sub>2</sub>O is suitable for optoelectronic devices.

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## 1. Introduction

Silver oxide (Ag<sub>2</sub>O) having direct band gap around 1.4 eV is a p-type semiconductor [1], used in optical memory [2], photography [3] and as solar energy converter [4]. It has been widely studied for its important roles in fast-ion-conducting glasses of the type AgI–Ag<sub>2</sub>O–B<sub>2</sub>O<sub>3</sub>, AgI–Ag<sub>2</sub>O–V<sub>2</sub>O<sub>5</sub>, and AgI–Ag<sub>2</sub>OP<sub>2</sub>O<sub>5</sub> [5,6]. Bond nature study between Ag and O is helpful to understand the ionic conduction mechanism and micro structure of glass [7]. Ag<sub>2</sub>O has cuprite structure (like Cu<sub>2</sub>O) with space group pn-3m (#224) [7]. We should emphasize that one of the main interesting properties of cuprite Ag<sub>2</sub>O is its negative thermal expansion behavior [8,9], another noteworthy property of Ag<sub>2</sub>O is the structural phase transition which occurs at about 35 K [10–12]. The purpose of present work is to study the structural, elastic, electronic, thermal, optical properties of Ag<sub>2</sub>O compound at ambient and under high pressure using the full-potential linearized augmented plane wave (FP-LAPW) method.

In the present paper, a brief introduction is given in Section 1. Method of calculation is presented in Section 2 of this paper. Results and discussions are given in Section 3 and finally concluding remarks are presented in Section 4.

## 2. Method of calculation

In this paper, we have calculated the Structural, elastic, electronic, and optical properties of Ag<sub>2</sub>O compound in the cuprite structure [7] at ambient and under pressure. These calculations are carried out within the framework of the density functional theory [13] using the full potential linearized augmented plane wave (FP-LAPW) [14] method, as implemented in the Wien2k Code [15]. We have used the local density approximation (LDA) [16], Generalized Gradient approximation (GGA) [17], Engel–Vosko generalized gradient approximation (EV–GGA) [18] and the modified Becke–Johnson exchange correlation potential plus Wu–Cohen version of generalized gradient approximation (mBJ–GGA). The mBJ exchange potential [19] was developed from a semi-local exchange potential proposed by Becke and Johnson (BJ-exchange potential) [20]. In the generalized gradient approximation (GGA) [17], the exchange correlation potential was treated for the self consistent calculations. Band structure calculations are carried out using LDA, GGA, EV–GGA and mBJ methods at 0–20 GPa pressure. The modified Becke–Johnson exchange potential (TB-mBJ) [19] yields very accurate electronic band structures and gaps for various types of semiconductors and insulators (e.g., sp semiconductors, noble-gas solids, and transition-metal oxides). As LDA and GGA underestimate band gaps and the electronic band dispersions, thus we will demonstrate the results obtained by mBJ–GGA–WC technique.

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In the FP-LAPW method, the wave function, charge density and potential are expanded in spherical harmonic functions inside muffin-tin spheres and by a plane-waves basis set in the interstitial region. Plane wave cut-off of  $K_{\text{MAX}} = 7.0/R_{\text{MT}}$  ( $R_{\text{MT}}$  is the plane wave radii, and  $K$ -max is the maximum modulus for the reciprocal lattice vectors) was chosen for  $\text{Ag}_2\text{O}$ . Values of muffin-tin radii ( $R_{\text{MT}}$ ) are considered to be equal to 1.94 and 1.72 Bohr for Ag and O respectively. In the non-overlapping muffin-tin spheres surrounding the atomic, the spherical harmonics are expanded up to  $l_{\text{max}} = 10$ . The charge density was Fourier expanded up to  $G_{\text{max}} = 12$  ( $\text{Ryd}$ )<sup>1/2</sup>. The band structures, electronic and optical calculations are carried out using a number of 1000  $k$ -points in the irreducible Brillouin zone (IBZ). The self consistent calculations are converged since the total energy of the system is stable within  $10^{-5}$  Ry.

### 3. Results and discussions

#### 3.1. Structural properties

Structural properties of  $\text{Ag}_2\text{O}$  compound are calculated using the volume optimization method. The total energy of  $\text{Ag}_2\text{O}$  is calculated using LDA, GGA and EV-GGA approaches. Volume optimization is performed by minimizing the total energy of the unit cell with respect to the volume of unit cell and total energy was calculated that fitted to the Murnaghan equation of state [21]. It is clear from Fig. 1, that using GGA method, initially energy of unit cell decreases with increase the volume of unit cell, the minimum energy state which is called the ground state energy  $E_0$  of the system is obtained. The volume at the ground state energy  $E_0$  is called the optimum volume or ground state volume of the system. After optimum volume point, the energy then increases with further increase in volume and the system is again in un-relaxed state. Moreover, the variations in lattice constant with the pressure between 0.0 and 20.0 GPa using LDA, GGA and EV-GGA approaches are depicted in Fig. 2. It can be seen from Fig. 2 that the lattice constant decreases with increase the pressure. Also, it is clear from Fig. 1 that using GGA method, the lattice constant ( $a_0 = 4.73$  Å) obtained at 0.0 GPa is in good agreement with available experimental data (4.74 Å) [22] and better than that calculated with LDA, EV-GGA and other theoretical results (4.83 Å) [22], (4.81 Å) [23]. As crystal rigidity is measured from Bulk modulus  $B_0$  and thus large value of  $B_0$  is responsible for high crystal rigidity. For  $\text{Ag}_2\text{O}$ , the calculated  $B_0$  is 86.73 GPa greater than 74.0 GPa [23] which show that the  $\text{Ag}_2\text{O}$  is soft semiconductor.

#### 3.2. Elastic properties

The elastic properties define the properties of materials, when it undergo stress, deform and then recover and return to its original

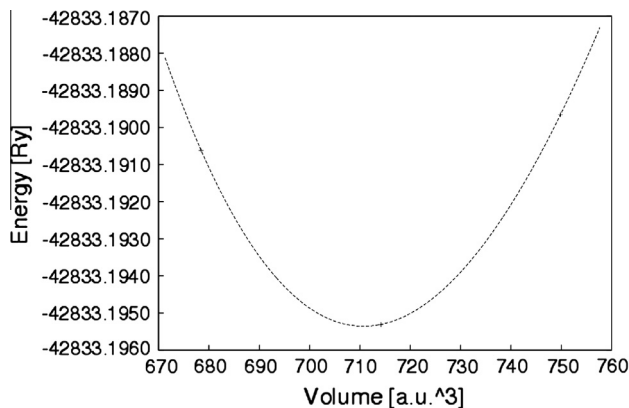


Fig. 1. Volume optimization curve for  $\text{Ag}_2\text{O}$ .

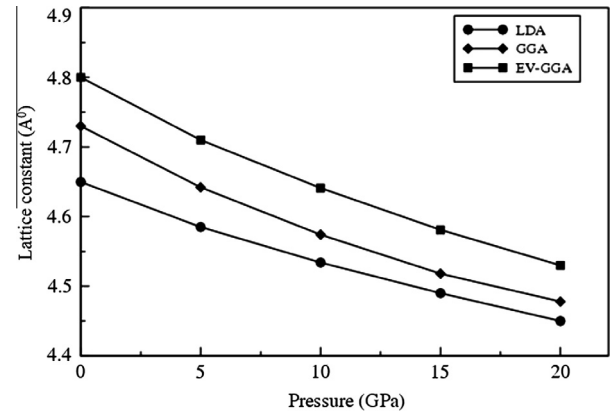


Fig. 2. Lattice constant (Å) versus Pressure (GPa) plot for  $\text{Ag}_2\text{O}$ .

shape after stress ceases. These properties play an important role in providing valuable information about binding characteristics between the adjacent atomic plane, structural stability, specific heat, thermal expansion, Debye temperature and many other properties.

Idea of elastic constants  $C_{ij}$  is important to study elastic nature of  $\text{Ag}_2\text{O}$ . Since  $\text{Ag}_2\text{O}$  has cubic symmetry therefore to understand and describe its mechanical behavior, we have calculated only three independent elastic parameters  $C_{11}$ ,  $C_{12}$  and  $C_{44}$ . Knowledge of these constants is helpful for information about stability and stiffness of materials. The calculated elastic parameters  $C_{11}$ ,  $C_{12}$  and  $C_{44}$  are 132.36, 70.94 and 56.18 GPa respectively. To the best of our knowledge there is no experimental data or theoretical results for the elastic properties of  $\text{Ag}_2\text{O}$  are available in the literature.

It is clear that  $C_{11}$ , which is related to the unidirectional compression along the principal crystallographic directions is greater than  $C_{44}$ , representing that  $\text{Ag}_2\text{O}$  offer a weaker resistance to the pure shear deformation compared to the resistance and to the unidirectional compression. Following restrictions are imposed on elastic constants in order to have mechanical stability in a cubic structure:

$$\frac{1}{3}(C_{11} + 2C_{12}) > 0; C_{44} > 0; \frac{1}{2}(C_{11} - C_{12}) > 0; C_{12} < B < C_{11} \quad (1)$$

Thus  $\text{Ag}_2\text{O}$  is elastically stable as satisfying these restrictions.

The elastic anisotropy ( $A$ ) has an important implication in industrial science to detect the micro cracks in materials. To detect micro cracks, we have calculated the anisotropy factor ( $A$ ) by  $A = 2C_{44}/(C_{11} - C_{12})$ . A material is completely isotropic for  $A = 1$  and anisotropic for any value less or greater than unity. As value of anisotropy factor is greater than unity (i.e.  $A = 1.829$ ). Hence,  $\text{Ag}_2\text{O}$  shows anisotropy.

We have applied the Voigt–Reuss–Hill approximation [24] to evaluate the Shear moduli ( $G$ ) from the elastic constants  $C_{ij}$ . For this purpose we have taken the arithmetic mean of the two well-known bounds for monocystals according to Voigt and Reuss [24–26]. In this way the moduli for the cubic structure are defined as:

$$G_V = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}) \quad (2)$$

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + (C_{11} - C_{12})} \quad (3)$$

$$B_V = B_R = \frac{(C_{11} + 2C_{12})}{3} \quad (4)$$

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