

# Investigation of Electronic, Elastic and Dynamic Properties of AgNbO<sub>3</sub> and AgTaO<sub>3</sub> under Pressure: Ab Initio Calculation

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How to cite this paper: Simsek, S. (2023) Investigation of Electronic, Elastic and Dynamic Properties of AgNbO<sub>3</sub> and AgTaO<sub>3</sub> under Pressure: Ab Initio Calculation. *World Journal of Condensed Matter Physics*, **13**, 57-77.

https://doi.org/10.4236/wjcmp.2023.132004

**Received:** April 2, 2023 **Accepted:** May 28, 2023 **Published:** May 31, 2023

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# Abstract

Based on the density functional theory within the local density approximation (LDA), we studied the electronic, elastic, and dynamic properties of AgNbO<sub>3</sub> and AgTaO3 compounds under pressure. The elastic constants, optic and static dielectric constants, born effective charges, and dynamic properties of AgNbO<sub>3</sub> and AgTaO<sub>3</sub> in cubic phase were studied as pressure dependences with the ab initio method. For these compounds, we have also calculated the bulk modulus, Young's modulus, shear modulus, Vickers hardness, Poisson's ratio, anisotropy factor, sound velocities, and Debye temperature from the obtained elastic constants. In addition, the brittleness and ductility properties of these compounds were estimated from Poisson's ratio and Pugh's rule (G/B). Our calculated values also show that AgNbO<sub>3</sub> (0.37) and AgTaO<sub>3</sub> (0.39) behave as ductile materials and steer away from brittleness by increasing pressure. The calculated values of Vicker hardness for both compounds indicate that they are soft materials. The results show that band gaps, elastic constants, elastic modules, and dynamic properties for both compounds are sensitive to pressure changes. We have also made some comparisons with related experimental and theoretical data that is available in the literature.

# **Keywords**

Electronic Structure, Elastic Constants, Born Effective Charges, Dynamic Properties, AgNbO<sub>3</sub>, AgTaO<sub>3</sub>

# **1. Introduction**

Silver niobate AgNbO<sub>3</sub> and silver tantalate AgTaO<sub>3</sub> are perovskite compounds that have not been intensively studied apart from structural phase transitions

and dielectric measurements, contrary to other perovskites such as BaTiO<sub>3</sub>, Ba-TaO<sub>3</sub>, LiNbO<sub>3</sub>, LiTaO<sub>3</sub>, KNbO<sub>3</sub> and KTaO<sub>3</sub>. Most studies on AgNbO<sub>3</sub> and Ag-TaO<sub>3</sub> were focused on Raman scattering, structural phase transitions, and dielectric measurements. One of the first Raman measurements of AgNbO3 over a large temperature was performed by A. Kania et al. [1]. The space groups for calcined AgNbO3 powder were investigated from 24°C to 630°C. Pure AgNbO3 undergoes successive phase transitions from the ferroelectric orthorhombic phase (Pbcm) to the paraelectric orthorhombic phase (Cmcm) at 347°C, then to the tetragonal phase (P4/mbm) at 377°C, and finally to the cubic phase (Pm3m) at 530°C [2]. Dielectric and domain structure investigations (300 K - 750 K) have been carried out for ceramics and two types of single crystals of silver niobate AgNbO3. An additional phase of the orthorhombic symmetry has been found in the temperature range 630 K - 638 K [3]. Yashima et al. have successfully addressed the longstanding issue of the crystal structure of ferroelectric AgNbO<sub>3</sub>. Convergent-beam electron diffraction (CBED) measurements on a single domain region of AgNbO3 allow us to unambiguously identify its space group as non-centrosymmetric Pmc21 [4]. Although the crystal structures of AgMO<sub>3</sub> were similar to those of NaMO<sub>3</sub> (M: Nb, Ta), it is found that the band gaps of AgTaO<sub>3</sub> and AgNbO<sub>3</sub> were 3.4 and 2.8 eV, respectively, being 0.6 eV smaller than the band gaps of NaTaO<sub>3</sub> (4.0 eV) and NaNbO<sub>3</sub> (3.4 eV) [5]. It was found from the electronic band structure study, using the plane-wave-based density functional method, that a hybrid orbital of Ag 4d and O 2p formed a valence band at a more negative level than O 2p orbitals [5]. Arney et al. found that the measured optical bandgap sizes of the AgNbO<sub>3</sub> products were in the range of ~2.75 - 2.81 eV [6]. One of the first investigations of silver tantalate AgTaO<sub>3</sub> was performed by Francombe and Lewis, who determined an orthorhombic structure with a monoclinic distortion of the pseudo-cubic perovskite unit cell at room temperature [7]. Kugel et al. revealed that an additional structural phase transtion occurred at a low temperature, which was not clearly indicated by X-ray measurements, between 10 and 873 K, on a polydomain AgTaO<sub>3</sub> sample [8]. It was shown that  $AgTaO_3$  single crystals are sensitive to external stress. The uniaxial pressure shifts the phase transition temperature, causes an increase in the permittivity, and makes the anomaly more pronounced. These effects can reflect the influence of electrical conductivity. It was shown that AgTaO<sub>3</sub> can be used as an element in a non-piezoelectric pressure sensor [9]. Because of recent developments in telecommunications, electro-optics, and piezoelectric components, perovskite niobates and tantalates have been placed on a short list of functional materials for future technologies [10].

In this work, we aimed at providing some additional information to the existing data on the physical properties of AgNbO<sub>3</sub> and AgTaO<sub>3</sub> compounds by using ab initio energy calculations, and we especially focused on the electronic, elastic, and dynamic properties. The layout of this paper is given as follows: the method of calculation is given in Section 2; the results and their discussion are in Section 3. Finally, the summary and conclusion are given in Section 4.

### 2. Computational Methods

AgNbO<sub>3</sub> and AgTaO<sub>3</sub> have cubic perovskite structures that are represented by space group (No. 221). There are five atoms in the cubic unit cell, and the lattice parameters for both compounds are given in **Table 1**. The electronic, elastic, and dynamic properties of AgNbO<sub>3</sub> and AgTaO<sub>3</sub> were theoretically studied by means of first principles calculations in the framework of density functional theory (DFT) and based on the local density approximation (LDA) [11] as implemented in the ABINIT code [12] [13]. The self-consistent norm-conserving pseudopotentials are generated using the Troullier-Martins scheme [14] which is included in the Perdew-Wang [15] scheme as parameterized by Ceperly and Alder [16]. Pseudopotentials are generated using the following electronic configurations: For Ag, the  $4d^{10}5s^{1}$  electron states,  $4d^{1}5s^{1}$  electron states for Nb,  $6s^{2}5d^{3}$  electron states for Ta, and  $2s^{2}2p^{4}$  electron states for O are considered the true valence. For calculations, the wave functions were expanded in plane waves up to a kinet-ic-energy cutoff of 40 Ha for AgNbO<sub>3</sub> and AgTaO<sub>3</sub>. The Brillouin zone was sampled using an  $8 \times 8 \times 8$  Monkhorst-Pack [17] mesh of special k points.

#### 3. Results and Discussion

#### **3.1. Structural Parameters**

As a first step of our study, we determined structural parameters using experimental data for  $AgNbO_3$  [2] and  $AgTaO_3$  [8]. The theoretical lattice parameters were obtained by minimizing the ratio of the total energy of the crystal to its volume, are given in **Table 1**. Then, lattice constants were carried out as dependence pressures in the range from 0 to 15 GPa, and all calculations were performed using these theoretical lattice parameters. Our structural estimation is in agreement with the available experimental and theoretical data (see **Table 1**).

Material	Reference	a (Å)	$E_g(eV)$	$C_{11}$	$C_{12}$	$C_{44}$	В	G	Ε
	LDA <sup>cal.</sup>	3.9468	1.63	513.3	107	49.1	242	90	241
	LDA [18]	3.9584	1.53						
	LDA [19]	3.9530	1.34						
AgNbO <sub>3</sub>	GGA [20]	3.9790	1.51						
	GGA [21]	3.9929	1.40				190		
	GGA [22]	3.9510	1.60				210		
	Exp. [2]	3.9598	2.8						
	LDA <sup>cal.</sup>	3.9537	2.22	530.8	105.2	53.5	247	97	257
	LDA [18]	3.9545	1.54						
A -T-O	LDA [23]	3.9490	1.53						
Ag1aO <sub>3</sub>	GGA [21]	3.9929	2.08				190		
	GGA [22]	3.9588	1.64				219		
	Exp. [8]	3.9484	3,4						

**Table 1.** The calculated equilibrium lattice parameters, band gaps, elastic constants, bulk modulus, shear modulus, and Young's modulus, together with the theoretical and experimental values for AgNbO<sub>3</sub> and AgTaO<sub>3</sub>.

#### **3.2. Electronic Properties**

The electronic band structures of AgNbO3 and AgTaO3 have been calculated in high-symmetry directions in the first Brillouin zone. The band structures and total (DOS) and partial (PDOS) densities of states for cubic AgNbO<sub>3</sub> and AgTaO<sub>3</sub> are shown in Figure 1 and Figure 2. As seen in Figure 1 and Figure 2 the Fermi level (EF) is set at zero energy and specified by a horizontal dashed red line. High-symmetry points in the Brillouin zone include  $\Gamma(0, 0, 0)$ , X (0, 1/2, 0), M (1/2, 1/2, 0) and R(1/2, 1/2, 1/2). The calculated electronic band structures for both crystals are similar. It is clear for both crystals that the band gap appears between the top-most valence band at M-point and the bottom-most conduction band at X-point for AgNbO<sub>3</sub> and Γ-point for AgTaO<sub>3</sub>. Accordingly, both AgNbO<sub>3</sub> and AgTaO<sub>3</sub> have an indirect band gap. The calculated indirect band gap values for AgNbO3 and AgTaO3 are 1.63 eV and 2.22 eV, respectively. We have found indirect band gaps of 1.533 eV for AgNbO3 and 1.537 eV for AgTaO3 in ours previous study [18]. These calculated values may also be smaller than experimental values because it is well known that the band gap calculated by DFT is smaller than that obtained from experiments. DFT generally underestimates the band gap in semiconductors and insulators [24]. The calculated equilibrium lattice parameters and band gaps, together with the theoretical and experimental values for AgNbO<sub>3</sub> and AgTaO<sub>3</sub> are given in Table 1. The calculated band gap values for these compounds are in good agreement with other DFT results, as shown in Table 1. We also calculated the influence of external pressure on the band gaps of AgNbO<sub>3</sub> and AgTaO<sub>3</sub>, which is given in Figure 3. The calculations show that direct band gaps increase linearly as a function of pressure for both compounds, but indirect band gaps do not change much with pressure. It is well known that



**Figure 1.** The calculated electronic band structure of AgNbO<sub>3</sub> (a) and AgTaO<sub>3</sub> (b) in cubic structure.



**Figure 2.** The calculated total DOS and partial PDOS for AgNbO<sub>3</sub> (a) and AgTaO<sub>3</sub> (b) in cubic structure.



**Figure 3.** Pressure dependence of the calculated direct (a) and indirect (b) band gaps of AgNbO<sub>3</sub> and AgTaO<sub>3</sub>.

the influence of pressure on  $E_g$  for most materials in a wide pressure range is linear ( $E_g = E_g(0) + AP + \cdots$ ). Our calculations show that  $A = 1.32 \times 10^{-3} \text{ eV/GPa}$  (AgNbO<sub>3</sub>) and  $1.64 \times 10^{-3} \text{ eV/GPa}$  (AgTaO<sub>3</sub>) for direct optical transition in the X-high symmetry point,  $6.47 \times 10^{-3} \text{ eV/GPa}$  (AgTaO<sub>3</sub>, between M- $\Gamma$  high symmetry points), and  $1.98 \times 10^{-3} \text{ eV/GPa}$  (AgNbO<sub>3</sub>, between M-X high symmetry points) for indirect transition.

To further clarify the nature of the electronic band structure of AgNbO<sub>3</sub> and AgTaO<sub>3</sub>, we have also calculated the total (DOS) and partial (PDOS) density of states, as shown in Figure 2(a) and Figure 2(b). As can be seen in Figure 2(a) and Figure 2(b), the DOS and PDOS for both crystals are quite similar. In both crystals, the bottom band between about -18 eV and -16 eV contains three valance bands that originate from O 2s orbital. In the calculated electronic band structure of AgNbO<sub>3</sub> and AgTaO<sub>3</sub> (see Figure 1(a) and Figure 1(b)), between

-6 eV and Fermi level (zero) there are fourteen valence bands. While Ag 4d orbitals between -6 and -5 eV are localized, the top of the valence band between -5 and 0 eV mainly consists of the oxygen O 2p states hypridized with Nb 4d and Ta 5d states for AgNbO<sub>3</sub> and AgTaO<sub>3</sub> respectively. The top of the valence band is mainly formed O 2p. In general, in perovskite compounds such as NaNbO<sub>3</sub>, *i.e.*, in perovskite compounds having an A-site atom without d orbital electrons, the top of the valence band consists of only O 2p constituents, and the orbital component of Na at the A-site does not appear in the valence band [20]. It is found to be in good agreement with the valence band width of AgNbO<sub>3</sub> calculated by A. Shigemi [20]. In cubic phase for both crystals, the fourteen valence bands at  $\Gamma$  point are separated into four triply degenerate levels and one doubly degenerate level. These splittings are produced by the crystal field and the electrostatic interaction between O 2p orbitals. In the conduction band, thirteen bands are split into two triply degenerate levels and two doubly degenerate levels.

#### **3.3. Elastic Properties**

Elastic constants are the most important characteristics of solids, and their knowledge is essential to understanding many of their properties. Elastic constants, in particular, determine the elasticity and mechanical stability of crystals. There is considerable interest in the elastic properties of the high-pressure phases of distinct crystals. An accurate experimental determination of elastic constants under pressure is often rather difficult, and here computer modeling can play an important role in establishing the properties of specific phases. Many response properties of materials can be calculated using the method of density function pertubation theory [25] [26]. There are three kinds of perturbation, such as electric field, atomic displacement, and strain, that were recently included in the ABINIT package [27]. By treating different perturbations, it can be calculated quantities such as elastic constants, born effective charges, piezoelectric coefficients, optical dielectric constants, and static dielectric constants. In this work, elastic constants, born effective charges, dielectric constants, and the phonon spectrum were calculated directly by applying atomic-displacement and electric-field perturbations. For cubic crystals, there are only three independent elastic constants, such as  $C_{11}$ ,  $C_{12}$  and  $C_{44}$ . From knowledge of elastic constants, other quantities can be calculated, such as bulk modulus (B), shear modulus (G), Young's modulus (E), and Poisson's ratio ( $\nu$ ). Mechanical stability leads to restrictions on the elastic constants, which for cubic crystal are [28],

$$C_{11} > 0, \ C_{44} > 0, \ C_{11} > |C_{12}|, \ (C_{11} + 2C_{12}) > 0, \ C_{12} < B < C_{11}$$
(1)

It is well known that shear modulus and bulk modulus are measures of the hardness of a solid. The bulk modulus is a measure of resistance to volume change by an applied pressure, whereas the shear modulus is a measure of resistance to reversible deformations upon shear stress [29]. Accordingly, the isotropic shear modules determine hardness better than the bulk modulus. For cubic crystal structure, the bulk modulus *B* and the shear modulus *G* are given [30]

[31] [32],

$$B = B_V + B_R = \frac{C_{11} + 2C_{12}}{3} \tag{2}$$

$$G_V = \frac{1}{5} \left( 2C + 3C_{44} \right) \tag{3}$$

$$G_R = \frac{15}{6/C + 9/C_{44}} \tag{4}$$

where  $B_V$  and  $G_V$  represent the Voigt bulk modulus and the shear modulus respectively, and  $B_R$  and  $G_R$  the Reuss bulk modulus and the shear modulus, respectively.

$$C = \frac{1}{2} (C_{11} - C_{12}) \tag{5}$$

According to the Voigt-Reuss-Hill approximation [33],

$$G = \left(G_V + G_R\right)/2 \tag{6}$$

Young's modules E and Poisson's ratio v can be obtained by

$$E = \frac{9BG}{3B+G}, \quad v = \frac{1}{2} \left( 1 - \frac{E}{3B} \right)$$
(7)

The Debye Temperature may be obtained from the average sound velocity  $V_m$  [34],

$$\Theta_D = \frac{\hbar}{k} \left[ \frac{3n}{4\pi} \left( \frac{N_A \rho}{M} \right) \right]^{1/3} V_m \tag{8}$$

where  $\hbar$  is Planck's constant, k is Boltzmann's constant,  $N_A$  is Avagadro's number, n is the number of atoms per formula unit, M is the molecular mass per formula unit,  $\rho$  is the density, and  $V_m$  is obtained from following Equation (9),

$$V_m = \left[\frac{1}{3} \left(\frac{2}{V_t^3} + \frac{1}{V_l^3}\right)\right]^{-1/3}$$
(9)

where  $V_t$  and  $V_l$  are the transverse and the longitudinal elastic wave velocities, respectively, which can be calculated from Navir's equations [35],

$$V_r = \sqrt{\frac{G}{\rho}} \tag{10}$$

$$V_l = \sqrt{\frac{3B + 4G}{3\rho}} \tag{11}$$

The calculated elastic constants, bulk modulus (*B*), shear modulus (*G*), and Young's modulus (*E*), for AgNbO<sub>3</sub> and AgTaO<sub>3</sub> are listed in **Table 1**. The pressure dependence of the calculated elastic constants, bulk modulus (*B*), shear modulus (*G*), and Young's modulus (*E*), for AgNbO<sub>3</sub> and AgTaO<sub>3</sub> is given in **Figure 4**. It can be seen from **Table 1** that our calculated values also satisfy all stability conditions (see ref [28]), as denoted by Equation (1).  $C_{11}$  elastic constant shows resistance to linear compression along x – y- or z-axes of the crystal, while

 $C_{12}$  and  $C_{44}$  elastic constants are related to the flexibility of the crystal. The values for AgTaO<sub>3</sub> are bigger than AgNbO<sub>3</sub>. Therefore, AgTaO<sub>3</sub> is more resistant than AgNbO<sub>3</sub> against linear compression along x - y- or z-axes of the crystal. We can obviously see from Figure 4(a) and Figure 4(b) that the  $C_{11}$  elastic constant increases with pressure dependence but  $C_{12}$  and  $C_{44}$  does not change much with pressure. The bulk modulus values for AgNbO3 and AgTaO3 were found to be 242 GPa and 247 GPa, respectively. As seen in Table 1, our calculated values for both compounds are close to the calculated values using GGA in WIEN2K software by A. Mahmood [22]. As seen from Figure 4(c) and Figure 4(d), bulk modulus (B), shear modulus (G), and Young's modulus (E) also have a trend to increase with increasing pressure for both compounds. However, the bulk modulus and Young's modulus for both compounds are more sensitive to the change in pressure compared to the shear modulus. We could not compare our results to the literature since there are no experimental and theoretical data on elastic constants, shear modulus (G), Young's modulus (E), and Poisson's ratio ( $\nu$ ) for both compounds.

To understand the nature of the anisotropy of both compounds, the profiles of the 2D and 3D planar projection plots of the elastic modulus and constants were drawn [35] and given in **Figure 5** and **Figure 6**. In these figures, minimum values are shown in green and maximum values in blue. The completely circular (2D) and spherical (3D) profiles indicate isotropy, while deviations from spherical and circular shapes reflect the degree of anisotropy in elastic modulus and constants of solids. Since AgNbO<sub>3</sub> and AgTaO<sub>3</sub> have the same cubic symmetry, their graphics are quite similar. **Figure 5** and **Figure 6(a)** demonstrate the anisotropy in compressibility (K). Due to a perfectly circular presentation of K on the xy, xz, and yz planes, K shows isotropic behavior for both compounds. The



**Figure 4.** Pressure dependence of the calculated elastic constants and elastic modulus of AgNbO<sub>3</sub> (a, c) and AgTaO<sub>3</sub> (b, d).



Figure 5. 2D and 3D representation of compressibility (a), Young's modulus (b), shear modulus (c) and Poission's ratio (d) for AgNbO<sub>3</sub>.

direction dependence of Young's modulus (E) is given in Figure 5 and Figure 6(b). It can be seen from Figure 5 and Figure 6(b) that the anisotropy of Young's modulus (E) on the xy, xz, and yz planes indicates anisotropic behavior



Figure 6. 2D and 3D representation of compressibility (a), Young modulu (b), shear modulu (c) and Poission's ratio (d) for Ag-TaO<sub>3</sub>.

due to a perfectly circular deviation. The maximum values of Young's modulus are 476.28 GPa and 496 GPa for AgNbO<sub>3</sub> and AgTaO<sub>3</sub>, respectively, while the minimum values of Young's modulus are 137.98 GPa and 149.69 GPa for AgN-

 $bO_3$  and AgTaO\_3. Like Young's modulus, as seen from Figure 5 and Figure 6(c), the shear modulus for both compounds displays anisotropic behavior. The largest value and the minimal value of shear modulus for AgNbO<sub>3</sub> (AgTaO<sub>3</sub>) is 203.1 (212.8) GPa and 49.1 (53.5) GPa, respectively. On the other hand, it can be seen from Figure 5 and Figure 6(d) that anisotropy is observed in the Poission's ratios of AgNbO<sub>3</sub> and AgTaO<sub>3</sub>.

Another way to identify the hardness of materials is to calculate the Vickers hardness ( $H_V$ ). Vickers hardness can be obtained from the calculated bulk modulus and shear modulus according to the following relation [36]:

$$H_{V} = 0.92 \left(\frac{G}{B}\right)^{1.137} G^{0.708}$$
(12)

The obtained Vickers hardnesses of AgNbO<sub>3</sub> and AgTaO<sub>3</sub> are 7.23 GPa and 8.11 GPa, respectively. If Vickers hardness is less than 10 GPa, it is defined as a soft material [37]. If Vickers hardness is greater than 40 GPa, then it is defined as a superhard material [38]. Because their Vickers hardness is smaller than 10 GPa, these compounds can be characterized as soft materials. The change with pressure of the Vickers hardness for AgNbO<sub>3</sub> and AgTaO<sub>3</sub> is given in Figure 7.

Poisson's ratio (v) has values in the range 0 < v < 0.5. The experimental values for most materials are close to 0.3 but, in any case, are always within the above limits [39]. We have found that Poisson's ratios are 0.334 and 0.327 for AgNbO<sub>3</sub> and AgTaO<sub>3</sub>, respectively. Our calculated values are within this limit. The values of the Poisson's ratio also reflect the degree of covalent bonding. The value of Poisson's is 0.25 for ionic materials, meanwhile v is 0.1 for covalently bonded materials [40]. Therefore, ionic contribution to inter atomic bonding for these compounds is more dominant. Besides, we clearly see from **Table 2** and **Table 3** that the values of the Poisson's are increasing by increasing pressure for both materials. On the other hand, as stated Pugh [41], if G/B > 0.5, the materials behave in a brittleness manner or if G/B < 0.5, the materials then become a ductile. Our calculated values show that AgNbO<sub>3</sub> (0.37) and AgTaO<sub>3</sub> (0.39) behave as ductile materials, and steer away from brittleness by increasing pressure.



**Figure 7.** Pressure dependence of the Vickers hardness of AgNbO<sub>3</sub> and AgTaO<sub>3</sub>.

Pressure (GPa)	ν	G/B	Α	$A^U$
0.0	0.334	0.37	0.16	2.85
2.5	0.337	0.36	0.15	3.08
5.0	0.340	0.35	0.14	3.51
7.5	0.342	0.35	0.13	3.64
10.0	0.344	0.34	0.13	3.89
12.5	0.347	0.34	0.12	4.34
15.0	0.348	0.33	0.12	4.49

**Table 2.** The calculated Poisson's ratio ( $\nu$ ), *G*/*B* ratios, Zener anisotropy factors *A* and, universal elastic anisotropy index  $A^U$  of AgNbO<sub>3</sub> under pressure.

**Table 3.** The calculated Poisson's ratio ( $\nu$ ), G/B ratios, Zener anisotropy factors A and, universal elastic anisotropy index  $A^U$  of AgTaO<sub>3</sub> under pressure.

Pressure (GPa)	ν	G/B	Α	$A^U$
0.0	0.327	0.39	0.17	2.66
2.5	0.329	0.38	0.16	2.87
5.0	0.331	0.38	0.15	3.02
7.5	0.335	0.37	0.14	3.47
10.0	0.337	0.36	0.14	3.62
12.5	0.339	0.35	0.13	3.93
15.0	0.342	0.34	0.12	4.30

The Zener anisotropy factor, A, reflects the degree of elastic anisotropy in a material. The Zener anisotropy factor is 1 for a completely isotropic material. For cubic crystals, the Zener anisotropy factor is given by [42],

$$A = \frac{2C_{44}}{C_{11}C_{12}} \tag{13}$$

The Zener anisotropy factors for AgNbO<sub>3</sub> and AgTaO<sub>3</sub> were calculated according to pressure and listed in **Table 2** and **Table 3**. The calculated Zener anisotropy factors for AgNbO<sub>3</sub> (0.16) and AgTaO<sub>3</sub> (0.17) are smaller than 1, which indicates that these compounds are entirely anisotropic. For these compounds, it can be seen from **Table 2** and **Table 3** that the Zener anisotropy factors decrease with increasing pressure.

Another important anisotropy factor that allows us to define elastic anisotropy py is the universal elastic anisotropy index,  $A^{U}$ . The universal elastic anisotropy index has zero for a completely isotropic material. The different values from zero of  $A^{U}$  state that material is anisotropic. The universal elastic anisotropy index can be calculated using the following equation [43].

$$A^{U} = 5G_{V}/G_{R} + B_{V}/B_{R} - 6$$
(14)

The obtained results are given in Table 2 and Table 3. As can be seen from Table 2 and Table 3, these compounds are anisotropic, and  $AgNbO_3$  is more

anisotropic than  $AgTaO_3$ . We can see from Table 2 and Table 3 that the universal elastic anisotropy index for both compounds has also trended to increase with increasing pressure.

We have also calculated Debye temperature, transverse, longitudinal, average sound velocities, and density implementing pressure from 0 to 15 GPa, which are shown in **Table 4** and **Table 5**. The Debye temperature is an important fundamental parameter since it is closely associated with many physical properties of materials, such as specific heat and melting temperature. The vibrational excitations originate purely from acoustic vibrations at low temperatures. Therefore, the Debye temperature obtained from elastic constants at low temperatures is the same as that determined from specific heat measurements. As seen in **Table 4** and **Table 5**, Debye temperature, transverse, longitudinal, average sound velocities, and density increase as dependent pressure. The Depye temperature, longitudinal, and average sound velocities of AgNbO<sub>3</sub> are higher than those of AgTaO<sub>3</sub>, but the calculated density of AgTaO<sub>3</sub> is higher than that of AgNbO<sub>3</sub>. Unfortunately, we could not find theoretical and experimental results in literature to compare with the Debye temperature, transverse, longitudinal, and average sound velocities.

**Table 4.** The density, transverse, longitudinal, and average elastic wave velocities, together with the Debye temperature of AgNbO<sub>3</sub> under pressure.

Pressure (GPa)	ho (g/cm <sup>3</sup> )	$v_t$ (m/s)	$v_l(m/s)$	$v_m$ (m/s)	Θ (K)
0.0	6.722	3670.24	7350.29	4117.65	530.78
2.5	6.789	3691.34	7435.43	4142.71	535.81
5.0	6.855	3685.25	7489.38	4137.97	536.91
7.5	6.918	3731.87	7607.21	4191.03	545.46
10.0	6.979	3747.57	7679.01	4209.88	549.52
12.5	7.039	3725.63	7702.04	4187.24	548.12
15.0	7.097	3776.17	7823.53	4244.54	557.14

**Table 5.** The density, transverse, longitudinal, and average elastic wave velocities, together with the Debye temperature of AgTaO<sub>3</sub> under pressure.

Pressure (GPa)	ho (g/cm <sup>3</sup> )	$v_t$ (m/s)	<i>v</i> <sub>2</sub> (m/s)	<i>v<sub>m</sub></i> (m/s)	Θ (K)
0.0	8.193	3438.78	6776.69	3854.25	495.96
2.5	8.274	3456.39	6848.18	3875.27	500.30
5.0	8.352	3497.45	6954.03	3922.12	507.94
7.5	8.428	3477.02	6978.31	3901.39	506.78
10.0	8.501	3506.62	7061.54	3935.35	512.67
12.5	8.572	3502.88	7099.82	3932.60	513.74
15.0	8.642	3500.93	7143.26	3931.89	515.03

# 3.4. Born Effective Charges, Dielectric Constants and Phonon Spectra

For periodic solids, the Born effective charge of an atom  $\kappa$  is tensor defined as the coefficient of proportionality at the linear order and under the condition of the zero macroscopic electric field, between the macroscopic polarization per unit cell created in direction  $\beta$  and a cooperative displacement of atoms  $\kappa$  in direction  $\alpha$ :

$$Z_{\kappa,\alpha\beta}^{*} = \Omega_{0} \frac{\partial \mathcal{P}_{\beta}}{\partial \tau_{\kappa,\alpha}} \bigg|_{\varepsilon=0}$$
(21)

where  $\Omega_0$  is the unit cell volume. The Born effective charge is a dynamic concept in the sense that it concerns the response to an atomic displacement. From its definition,  $Z^*$  is a fundamental quantity in lattice dynamics: it governs, with the optical dielectric constant  $\varepsilon_{\infty}$ , the strength of the Coulomb interaction responsible for the splitting between longitudinal (LO) and transverse (TO) optic modes [44].

The calculated Born effective charges  $Z^*$ , optical dielectric constant  $\varepsilon_{\infty}$ , and static dielectric constant  $\varepsilon_s$  of AgNbO<sub>3</sub> and AgTaO<sub>3</sub> under pressure are given in Table 6 and in Table 7. In the cubic phase, they are explicitly described by a set of four independent numbers for ABO3 compounds. The charge of A and B atoms is isotropic, since their atomic positions have local spherical symmetry. For the oxygen atom, there are two independent elements  $O_{\parallel}$  and  $O_{\perp}$  that must be taken into consideration, parallel and perpendicular to the B-O bond. As seen from **Table 6** and **Table 7**, while  $Z_{Ag}^*$ ,  $Z_{Nb}^*$  and  $Z_{Ta}^*$  tensors are isotropic,  $Z_{O}^{*}$  tensors are highly anisotropic. We see that  $Z_{Nb}^{*}$ ,  $Z_{Ta}^{*}$  and  $Z_{O_{1}}^{*}$ significantly deviate from their nominal ionic values (+5 for Nb, +5 for Ta, and -2 for O). It reflects the sensitivity to atomic displacement of the partially covalent nature of the Nb-O and Ta-O bonds [45]. However,  $Z_{Ag}^*$  and  $Z_{O_{\parallel}}^*$  are close to their ionic charges. This implies that the bond between Ag and O is weakly covalent [2]. On the other hand, charge neutrality, reflecting the numerical accuracy of our calculation, is fulfilled to within 10<sup>-3</sup>. We see from Table 6 and **Table 7** that the values of  $Z_{Ag}^*$ ,  $Z_{Nb}^*$ ,  $Z_{Ta}^*$  and  $Z_{O_{\perp}}^*$  decrease as pressure increases, whereas  $Z_{O_{1}}^{*}$  increase with increasing pressure. We also calculated the optical dielectric constant ( $\varepsilon_{\infty}$ ) and static dielectric constant ( $\varepsilon_s$ ) of AgNbO<sub>3</sub> and AgTaO<sub>3</sub> as pressure dependence. Because of the symmetry of the crystal, the optical dielectric constant and static dielectric constant of AgNbO3 and AgTaO3 have only one component in cubic phase. As seen from Table 6 and Table 7, there is also a trend to decrease with increasing pressure.

Since AgNbO<sub>3</sub> and AgTaO<sub>3</sub> have ideal cubic perovskite structures (space groups  $O_h^1$ , Pm3m), there are 15 normal modes of vibration. These modes are shown at the zone center as following irreducible representations.

$$\Gamma(O_h^1) = 4F_{1u} + F_{2u} \tag{22}$$

P(GPa)	$Z^*_{\scriptscriptstyle Ag}$	$Z^*_{\scriptscriptstyle Nb}$	$Z_{o_1}^*$	$Z_{O2}^*$	$Z_{O3}^{*}$	$\mathcal{E}_{\infty}$ $\mathcal{E}_{s}$
nominal	1	5	-2	-2	-2	
0	$\begin{pmatrix} 1.583 & 0 & 0 \\ 0 & 1.583 & 0 \\ 0 & 0 & 1.583 \end{pmatrix}$	$\begin{pmatrix} 9.359 & 0 & 0 \\ 0 & 9.359 & 0 \\ 0 & 0 & 9.359 \end{pmatrix}$	$\begin{pmatrix} -1.906 & 0 & 0 \\ 0 & -1.906 & 0 \\ 0 & 0 & -7.129 \end{pmatrix}$	$\begin{pmatrix} -1.906 & 0 & 0 \\ 0 & -7.129 & 0 \\ 0 & 0 & -1.906 \end{pmatrix}$	$ \begin{pmatrix} -7.129 & 0 & 0 \\ 0 & -1.906 & 0 \\ 0 & 0 & -1.906 \end{pmatrix} $	7.51 87.67
2.5	$\begin{pmatrix} 1.581 & 0 & 0 \\ 0 & 1.581 & 0 \\ 0 & 0 & 1.581 \end{pmatrix}$	$\begin{pmatrix} 9.350 & 0 & 0 \\ 0 & 9.350 & 0 \\ 0 & 0 & 9.350 \end{pmatrix}$	$\begin{pmatrix} -1.907 & 0 & 0 \\ 0 & -1.907 & 0 \\ 0 & 0 & -7.116 \end{pmatrix}$	$\begin{pmatrix} -1.907 & 0 & 0 \\ 0 & -7.116 & 0 \\ 0 & 0 & -1.907 \end{pmatrix}$	$\begin{pmatrix} -7.116 & 0 & 0 \\ 0 & -1.907 & 0 \\ 0 & 0 & -1.907 \end{pmatrix}$	7.48 80.21
5.0	$\begin{pmatrix} 1.579 & 0 & 0 \\ 0 & 1.579 & 0 \\ 0 & 0 & 1.579 \end{pmatrix}$	$\begin{pmatrix} 9.341 & 0 & 0 \\ 0 & 9.341 & 0 \\ 0 & 0 & 9.341 \end{pmatrix}$	$\begin{pmatrix} -1.908 & 0 & 0 \\ 0 & -1.908 & 0 \\ 0 & 0 & -7.103 \end{pmatrix}$	$\begin{pmatrix} -1.908 & 0 & 0 \\ 0 & -7.103 & 0 \\ 0 & 0 & -1.908 \end{pmatrix}$	$\begin{pmatrix} -7.103 & 0 & 0 \\ 0 & -1.908 & 0 \\ 0 & 0 & -1.908 \end{pmatrix}$	7.45 75.90
7.5	$\begin{pmatrix} 1.578 & 0 & 0 \\ 0 & 1.578 & 0 \\ 0 & 0 & 1.578 \end{pmatrix}$	$\begin{pmatrix} 9.334 & 0 & 0 \\ 0 & 9.334 & 0 \\ 0 & 0 & 9.334 \end{pmatrix}$	$\begin{pmatrix} -1.909 & 0 & 0 \\ 0 & -1.909 & 0 \\ 0 & 0 & -7.092 \end{pmatrix}$	$\begin{pmatrix} -1.909 & 0 & 0 \\ 0 & -7.092 & 0 \\ 0 & 0 & -1.909 \end{pmatrix}$	$\begin{pmatrix} -7.092 & 0 & 0 \\ 0 & -1.909 & 0 \\ 0 & 0 & -1.909 \end{pmatrix}$	7.42 73.74
10.0	$\begin{pmatrix} 1.576 & 0 & 0 \\ 0 & 1.576 & 0 \\ 0 & 0 & 1.576 \end{pmatrix}$	$\begin{pmatrix} 9.327 & 0 & 0 \\ 0 & 9.327 & 0 \\ 0 & 0 & 9.327 \end{pmatrix}$	$\begin{pmatrix} -1.910 & 0 & 0 \\ 0 & -1.910 & 0 \\ 0 & 0 & -7.082 \end{pmatrix}$	$\begin{pmatrix} -1.910 & 0 & 0 \\ 0 & -7.082 & 0 \\ 0 & 0 & -1.910 \end{pmatrix}$	$\begin{pmatrix} -7.082 & 0 & 0 \\ 0 & -1.910 & 0 \\ 0 & 0 & -1.910 \end{pmatrix}$	7.40 73.29
12.5	$\begin{pmatrix} 1.575 & 0 & 0 \\ 0 & 1.575 & 0 \\ 0 & 0 & 1.575 \end{pmatrix}$	$\begin{pmatrix} 9.321 & 0 & 0 \\ 0 & 9.321 & 0 \\ 0 & 0 & 9.321 \end{pmatrix}$	$\begin{pmatrix} -1.911 & 0 & 0 \\ 0 & -1.911 & 0 \\ 0 & 0 & -7.073 \end{pmatrix}$	$\begin{pmatrix} -1.911 & 0 & 0 \\ 0 & -7.073 & 0 \\ 0 & 0 & -1.911 \end{pmatrix}$	$\begin{pmatrix} -7.073 & 0 & 0 \\ 0 & -1.911 & 0 \\ 0 & 0 & -1.911 \end{pmatrix}$	7.38 74.45
15.0	$\begin{pmatrix} 1.573 & 0 & 0 \\ 0 & 1.573 & 0 \\ 0 & 0 & 1.573 \end{pmatrix}$	$\begin{pmatrix} 9.316 & 0 & 0 \\ 0 & 9.316 & 0 \\ 0 & 0 & 9.316 \end{pmatrix}$	$\begin{pmatrix} -1.912 & 0 & 0 \\ 0 & -1.912 & 0 \\ 0 & 0 & -7.065 \end{pmatrix}$	$\begin{pmatrix} -1.912 & 0 & 0 \\ 0 & -7.065 & 0 \\ 0 & 0 & -1.912 \end{pmatrix}$	$\begin{pmatrix} -7.065 & 0 & 0 \\ 0 & -1.912 & 0 \\ 0 & 0 & -1.912 \end{pmatrix}$	7.36 77.40

Table 6. Born effective charges, optical and static dielectric constants of AgNbO3 under pressure.

	Table 7. Born effective charges,	optical and static dielectric constants of A	gTaO3 under pressure.
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P(GPa)	$Z^*_{\scriptscriptstyle Ag}$	$Z^*_{Ta}$	$Z^*_{O1}$	$Z_{O2}^*$	$Z_{O3}^*$	$\mathcal{E}_{\infty}$	$\mathcal{E}_{s}$
nominal	1	5	-2	-2	-2		
0	$\begin{pmatrix} 1.572 & 0 & 0 \\ 0 & 1.572 & 0 \\ 0 & 0 & 1.572 \end{pmatrix}$	$\begin{pmatrix} 8.522 & 0 & 0 \\ 0 & 8.522 & 0 \\ 0 & 0 & 8.522 \end{pmatrix}$	$\begin{pmatrix} -1.882 & 0 & 0 \\ 0 & -1.882 & 0 \\ 0 & 0 & -6.329 \end{pmatrix}$	$\begin{pmatrix} -1.882 & 0 & 0 \\ 0 & -6.329 & 0 \\ 0 & 0 & -1.882 \end{pmatrix}$	$\begin{pmatrix} -6.329 & 0 & 0 \\ 0 & -1.882 & 0 \\ 0 & 0 & -1.882 \end{pmatrix}$	6.43	56.94
2.5	$\begin{pmatrix} 1.570 & 0 & 0 \\ 0 & 1.570 & 0 \\ 0 & 0 & 1.570 \end{pmatrix}$	$\begin{pmatrix} 8.519 & 0 & 0 \\ 0 & 8.519 & 0 \\ 0 & 0 & 8.519 \end{pmatrix}$	$\begin{pmatrix} -1.884 & 0 & 0 \\ 0 & -1.884 & 0 \\ 0 & 0 & -6.320 \end{pmatrix}$	$\begin{pmatrix} -1.884 & 0 & 0 \\ 0 & -6.320 & 0 \\ 0 & 0 & -1.884 \end{pmatrix}$	$\begin{pmatrix} -6.320 & 0 & 0 \\ 0 & -1.884 & 0 \\ 0 & 0 & -1.884 \end{pmatrix}$	6.41	53.25
5.0	$\begin{pmatrix} 1.568 & 0 & 0 \\ 0 & 1.568 & 0 \\ 0 & 0 & 1.568 \end{pmatrix}$	$\begin{pmatrix} 8.518 & 0 & 0 \\ 0 & 8.518 & 0 \\ 0 & 0 & 8.518 \end{pmatrix}$	$\begin{pmatrix} -1.887 & 0 & 0 \\ 0 & -1.887 & 0 \\ 0 & 0 & -6.312 \end{pmatrix}$	$\begin{pmatrix} -1.887 & 0 & 0 \\ 0 & -6.312 & 0 \\ 0 & 0 & -1.887 \end{pmatrix}$	$\begin{pmatrix} -6.312 & 0 & 0 \\ 0 & -1.887 & 0 \\ 0 & 0 & -1.887 \end{pmatrix}$	6.39	50.90
7.5	$\begin{pmatrix} 1.567 & 0 & 0 \\ 0 & 1.567 & 0 \\ 0 & 0 & 1.567 \end{pmatrix}$	$\begin{pmatrix} 8.517 & 0 & 0 \\ 0 & 8.517 & 0 \\ 0 & 0 & 8.517 \end{pmatrix}$	$\begin{pmatrix} -1.889 & 0 & 0 \\ 0 & -1.889 & 0 \\ 0 & 0 & -6.305 \end{pmatrix}$	$\begin{pmatrix} -1.889 & 0 & 0 \\ 0 & -6.305 & 0 \\ 0 & 0 & -1.889 \end{pmatrix}$	$\begin{pmatrix} -6.305 & 0 & 0 \\ 0 & -1.889 & 0 \\ 0 & 0 & -1.889 \end{pmatrix}$	6.38	49.52
10.0	$\begin{pmatrix} 1.565 & 0 & 0 \\ 0 & 1.565 & 0 \\ 0 & 0 & 1.565 \end{pmatrix}$	$\begin{pmatrix} 8.516 & 0 & 0 \\ 0 & 8.516 & 0 \\ 0 & 0 & 8.516 \end{pmatrix}$	$\begin{pmatrix} -1.891 & 0 & 0 \\ 0 & -1.891 & 0 \\ 0 & 0 & -6.299 \end{pmatrix}$	$\begin{pmatrix} -1.891 & 0 & 0 \\ 0 & -6.299 & 0 \\ 0 & 0 & -1.891 \end{pmatrix}$	$\begin{pmatrix} -6.299 & 0 & 0 \\ 0 & -1.891 & 0 \\ 0 & 0 & -1.891 \end{pmatrix}$	6.37	48.92
12.5	$\begin{pmatrix} 1.564 & 0 & 0 \\ 0 & 1.564 & 0 \\ 0 & 0 & 1.564 \end{pmatrix}$	$\begin{pmatrix} 8.515 & 0 & 0 \\ 0 & 8.515 & 0 \\ 0 & 0 & 8.515 \end{pmatrix}$	$\begin{pmatrix} -1.893 & 0 & 0 \\ 0 & -1.893 & 0 \\ 0 & 0 & -6.293 \end{pmatrix}$	$\begin{pmatrix} -1.893 & 0 & 0 \\ 0 & -6.293 & 0 \\ 0 & 0 & -1.893 \end{pmatrix}$	$\begin{pmatrix} -6.293 & 0 & 0 \\ 0 & -1.893 & 0 \\ 0 & 0 & -1.893 \end{pmatrix}$	6.36	48.99
15.0	$\begin{pmatrix} 1.562 & 0 & 0 \\ 0 & 1.562 & 0 \\ 0 & 0 & 1.562 \end{pmatrix}$	$\begin{pmatrix} 8.514 & 0 & 0 \\ 0 & 8.514 & 0 \\ 0 & 0 & 8.514 \end{pmatrix}$	$\begin{pmatrix} -1.895 & 0 & 0 \\ 0 & -1.895 & 0 \\ 0 & 0 & -6.288 \end{pmatrix}$	$\begin{pmatrix} -1.895 & 0 & 0 \\ 0 & -6.288 & 0 \\ 0 & 0 & -1.895 \end{pmatrix}$	$\begin{pmatrix} -6.288 & 0 & 0 \\ 0 & -1.895 & 0 \\ 0 & 0 & -1.895 \end{pmatrix}$	6.35	49.74

DOI: 10.4236/wjcmp.2023.132004

where one of the  $F_{1u}$  irreducible representations corresponds to a triple degenerate acoustical mode. The other three  $F_{1u}$  irreducible representations are the infrared (IR) active optical modes, which allow for cubic symmetry. The  $F_{2u}$  irreducible representation corresponds to a silent mode, which is neither IR nor Raman active [46].

The calculated phonon dispersion curves and total DOS and partial PDOS densities of states for cubic AgNbO3 and AgTaO3 are plotted along the highsymmetry directions in the first Brillouin in Figure 8 and Figure 9. Negative values in Figure 8(a) and Figure 8(b) represent imaginary frequencies. The phonon dispersion of the AgNbO<sub>3</sub> compound is similar to the phonon dispersion of AgTaO<sub>3</sub>. There are unstable modes along the direction X-M-R-Γ-M for both compounds, which determine the nature of the ferroelectric and antiferrodistortive phase transitions and the dielectric and piezoelectric responses of the compounds. For both compounds, there is also one triply soft mode degenerate level (171.8 cm<sup>-1</sup> for AgNbO<sub>3</sub> and 171.2 cm<sup>-1</sup> for AgTaO<sub>3</sub>) at the R point. Our results show that the unstable modes for AgNbO3 and AgTaO3 occupy a large place in the Brillouin zone. These soft modes have a flat dispersion along the direction X-M-R-Γ. We see in Figure 9(a) and Figure 9(b) that the motion of Ag, Nb, and Ta atoms is more irruption in the low-frequency region. The majority of phonon modes consist of O atoms at high frequencies. When analyzing the phonon DOS and PDOS of these compounds, we see that unstable modes originate from O atoms.



**Figure 8.** The calculated phonon band structure of AgNbO<sub>3</sub> (a) and AgTaO<sub>3</sub> (b).



**Figure 9.** The calculated phonon total DOS and partial PDOS of AgNbO<sub>3</sub> (a) and AgTaO<sub>3</sub> (b).

# 4. Conclusion

As a result, we have calculated the electronic structure, the total DOS and PDOS, the elastic constants, and the mechanical and vibrational properties of AgNbO3 and  $AgTaO_3$  using the density functional theory based on the ABINIT code. The electronic structure calculation showed that both compounds have an indirect (M-X for AgNbO<sub>3</sub> and M- $\Gamma$  for AgTaO<sub>3</sub>) band gap. The results show that the calculated band gaps of these compounds are pressure dependent. It was calculated mechanical and dynamical quantities such as born effective charges, dielectric constants, elastic constants, bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson's ratio ( $\nu$ ) and the Depye temperatures under pressure. The calculated elastic constants satisfy mechanical stability conditions. Our calculated values also show that AgNbO<sub>3</sub> (0.37) and AgTaO<sub>3</sub> (0.39) behave as ductile materials, and steer away from brittleness by increasing pressure. The values of Vicker hardness for both compounds indicate to be soft materials. The values of  $Z_{A_g}^*$ ,  $Z_{Nb}^*$ ,  $Z_{Ta}^*$  and  $Z_{O_1}^*$  decrease as a function of pressure, whereas  $Z_{O_1}^*$  increases with increasing pressure. We have also investigated the phonon band structures of AgNbO3 and AgTaO3 using the ab initio method. We determined that the unstable modes cause the ferroelectric, antiferrodistortive phase transitions and the dielectric and piezoelectric responses of the compounds.

### **Conflicts of Interest**

The author declares no conflicts of interest regarding the publication of this paper.

#### References

- Kania, A., Roleder, K., Kugel, G.E. and Fontana, M.D. (1986) Raman-Scattering, Central Peak and Phase-Transitions in AgNbO<sub>3</sub>. *Journal of Physics C—Solid State Physics*, 19, 9-20. <u>https://doi.org/10.1088/0022-3719/19/1/007</u>
- [2] Sciau, P., Kania, A., Dkhil, B., Suard, E. and Ratuszna, A. (2004) Structural Investigation of AgNbO<sub>3</sub> Phases Using X-Ray and Neutron Diffraction. *Journal of Physics—Condensed Matter*, **16**, 2795-2810. https://doi.org/10.1088/0953-8984/16/16/004
- [3] Kania, A. (1998) An Additional Phase Transition in Silver Niobate AgNbO<sub>3</sub>. Ferroelectrics, 205, 19-28. <u>https://doi.org/10.1080/00150199808228384</u>
- Yashima, M., Matsuyama, S., Sano, R., Itoh, M., Tsuda, K. and Fu, D.S. (2011) Structure of Ferroelectric Silver Niobate AgNbO<sub>3</sub>. *Chemistry of Materials*, 23, 1643-1645. <u>https://doi.org/10.1021/cm103389q</u>
- [5] Kato, H., Kobayashi, H. and Kudo, A. (2002) Role of Ag<sup>+</sup> in the Band Structures and Photocatalytic Properties of AgMO<sub>3</sub> (M: Ta and Nb) with the Perovskite Structure. *Journal of Physical Chemistry B*, **106**, 12441-12447. <u>https://doi.org/10.1021/ip025974n</u>
- [6] Arney, D., Hardy, C., Greve, B. and Maggard, P.A. (2010) Flux Synthesis of AgNbO<sub>3</sub>: Effect of Particle Surfaces and Sizes on Photocatalytic Activity. *Journal of Photochemistry and Photobiology A—Chemistry*, **214**, 54-60. <u>https://doi.org/10.1016/j.jphotochem.2010.06.006</u>
- [7] Schulze, G. (1963) F. Jona and G. Shirane, Ferroelectric Crystals. 402 S. Oxford/ London/New York/Paris 1962. Pergamon Press. Preis geb. 84 s. net. ZAMM— Journal of Applied Mathematics and Mechanics, 43, 512. https://doi.org/10.1002/zamm.19630431016
- [8] Kugel, G.E., Fontana, M.D., Hafid, M., Roleder, K., Kania, A. and Pawelczyk, M. (1987) A Raman-Study of Silver Tantalate (AgTaO<sub>3</sub>) and Its Structural Phase-Transition Sequence. *Journal of Physics C—Solid State Physics*, 20, 1217-1230. https://doi.org/10.1088/0022-3719/20/9/012
- [9] Suchanicz, J. and Kania, A. (2009) Uniaxial Pressure Effect on Dielectric Properties of AgTaO<sub>3</sub> Single Crystals. *Ferroelectrics*, **393**, 21-26. https://doi.org/10.1080/00150190903412614
- [10] Valant, M., Axelsson, A.K., Zou, B. and Alford, N. (2007) Strain Influence on Crystallography of AgNbO<sub>3</sub>-Based Thin Films. *Journal of Optoelectronics and Advanced Materials*, 9, 1377-1381.
- [11] Cohen, R.E. and Krakauer, H. (1990) Lattice-Dynamics and Origin of Ferroelectricity in Batio3—Linearized-Augmented-Plane-Wave Total-Energy Calculations. *Physi*cal Review B, 42, 6416-6423. <u>https://doi.org/10.1103/PhysRevB.42.6416</u>
- [12] Gonze, X., Beuken, J.M., Caracas, R., Detraux, F., Fuchs, M., et al. (2002) First-Principles Computation of Material Properties: The ABINIT Software Project. Computational Materials Science, 25, 478-492. https://doi.org/10.1016/S0927-0256(02)00325-7
- Fuchs, M. and Scheffler, M. (1999) *Ab Initio* Pseudopotentials for Electronic Structure Calculations of Poly-Atomic Systems Using Density-Functional Theory. *Computer Physics Communications*, **119**, 67-98. https://doi.org/10.1016/S0010-4655(98)00201-X
- [14] Troullier, N. and Martins, J.L. (1991) Efficient Pseudopotentials for Plane-Wave Calculations. *Physical Review B*, 43, 1993-2006.

https://doi.org/10.1103/PhysRevB.43.1993

- Perdew, J.P. and Wang, Y. (2018) Erratum: Accurate and Simple Analytic Representation of the Electron-Gas Correlation Energy [Phys. Rev. B 45, 13244 (1992)]. *Physical Review B*, 98, Article ID: 079904. https://doi.org/10.1103/PhysRevB.98.079904
- [16] Ceperley, D.M. and Alder, B.J. (1980) Ground-State of the Electron-Gas by a Stochastic Method. *Physical Review Letters*, **45**, 566-569. <u>https://doi.org/10.1103/PhysRevLett.45.566</u>
- [17] Monkhorst, H.J. and Pack, J.D. (1976) Special Points for Brillonin-Zone Integrations. *Physical Review B*, 13, 5188-5192. <u>https://doi.org/10.1103/PhysRevB.13.5188</u>
- [18] Cabuk, S. and Simsek, S. (2008) First-Principles Studies of the Electronic Structure and Optical Properties of AgBO<sub>3</sub> (B = Nb, Ta) in the Paraelectric Phase. *Central European Journal of Physics*, 6, 730-736. <u>https://doi.org/10.2478/s11534-008-0046-9</u>
- [19] Erdinc, B. and Kaval, M. (2017) DFT Study of Electronic and Optical Properties of Paraelectric AgNbO<sub>3</sub> Crystal under 0-50 GPa Pressure. *Indian Journal of Physics*, 91, 653-657. <u>https://doi.org/10.1007/s12648-017-0961-y</u>
- [20] Shigemi, A. and Wada, T. (2008) Crystallographic Phase Stabilities and Electronic Structures in AgNbO<sub>3</sub> by First-Principles Calculation. *Molecular Simulation*, 34, 1105-1114. <u>https://doi.org/10.1080/08927020802235698</u>
- [21] Prasad, K.G., Niranjan, M.K. and Asthma, S. (2016) The Structural and Electronic Properties of Cubic AgMO<sub>3</sub> (M = Nb, Ta) by First Principles Calculations. *AIP Conference Proceedings*, **1728**, Article ID: 020102. https://doi.org/10.1063/1.4946153
- [22] Mahmood, A., Ramay, S.M., Rafique, H.M., Al-Zaghayer, Y. and Khan, S.U.D. (2014) First-Principles Study of Electronic, Optical and Thermoelectric Properties in Cubic Perovskite Materials AgMO<sub>3</sub> (M = V, Nb, Ta). *Modern Physics Letters B*, 28, Article ID: 1450077. <u>https://doi.org/10.1142/S0217984914500778</u>
- [23] Erdinc, B. and Dede, M. (2016) First-Principles Study of Electronic and Optical Properties of Cubic AgTaO<sub>3</sub> Structure in Paraelectric Phase at Different Pressures. *Ferroelectrics*, **504**, 130-138. <u>https://doi.org/10.1080/00150193.2016.1240005</u>
- [24] Martin, R.M. (2020) Electronic Structure: Basic Theory and Practical Methods. Cambridge University Press, Cambridge. <u>https://doi.org/10.1017/9781108555586</u>
- [25] Gonze, X. (1995) Perturbation Expansion of Variational-Principles at Arbitrary Order. *Physical Review A*, **52**, 1086-1095.
   <u>https://doi.org/10.1103/PhysRevA.52.1086</u>
- [26] Baroni, S., de Gironcoli, S., Dal Corso, A. and Giannozzi, P. (2001) Phonons and Related Crystal Properties from Density-Functional Perturbation Theory. *Reviews* of Modern Physics, 73, 515-562. <u>https://doi.org/10.1103/RevModPhys.73.515</u>
- [27] Hamann, D.R., Wu, X., Rabe, K.M. and Vanderbilt, D. (2005) Metric Tensor Formulation of Strain in Density-Functional Perturbation Theory. *Physical Review B*, 72, Article ID: 035117.
- [28] Wu, Z.J., Zhao, E.J., Xiang, H.P., Hao, X.F., Liu, X.J. and Meng, J. (2007) Crystal Structures and Elastic Properties of Superhard IrN<sub>2</sub> and IrN<sub>3</sub> from First Principles. *Physical Review B*, **76**, Article ID: 054115.
- [29] Koc, H., Deligoz, E. and Mamedov, A.M. (2011) The Elastic, Electronic, and Optical Properties of PtSi and PtGe Compounds. *Philosophical Magazine*, **91**, 3093-3107. <u>https://doi.org/10.1080/14786435.2011.566229</u>
- [30] Kong, B., Zhu, B., Cheng, Y., Zhang, L., Zeng, Q.X. and Sun, X.W. (2011) Structur-

al, Mechanical, Thermodynamics Properties and Phase Transition of FeVSb. *Physica B—Condensed Matter*, **406**, 3003-3010. https://doi.org/10.1016/j.physb.2011.04.067

- [31] Voigt, W. (1910) Lehrbuch der kristallphysik: (Mit ausschluss der kristalloptik). BG Teubner, Berlin.
- [32] Reuss, A. (1929) Calculation of the Flow Limits of Mixed Crystals on the Basis of the Plasticity of Monocrystals. *Zeitschrift fur Angewandte Mathematik und Mechanik*, 9, 49-58. <u>https://doi.org/10.1002/zamm.19290090104</u>
- [33] Hill, R. (1952) The Elastic Behaviour of a Crystalline Aggregate. *Proceedings of the Physical Society. Section A*, 65, 349-354. https://doi.org/10.1088/0370-1298/65/5/307
- [34] Anderson, O.L. (1963) A Simplified Method for Calculating the Debye Temperature from Elastic Constants. *Journal of Physics and Chemistry of Solids*, 24, 909-917. <u>https://doi.org/10.1016/0022-3697(63)90067-2</u>
- [35] Gaillac, R., Pullumbi, P. and Coudert, F.X. (2016) ELATE: An Open-Source Online Application for Analysis and Visualization of Elastic Tensors. *Journal of Physics-Condensed Matter*, 28, Article ID: 275201. https://doi.org/10.1088/0953-8984/28/27/275201
- [36] Tian, Y.J., Xu, B. and Zhao, Z.S. (2012) Microscopic Theory of Hardness and Design of Novel Superhard Crystals. *International Journal of Refractory Metals & Hard Materials*, 33, 93-106. <u>https://doi.org/10.1016/j.ijrmhm.2012.02.021</u>
- [37] Liu, W.N., Niu, Y.T. and Li, W.Q. (2020) Theoretical Prediction of the Physical Characteristic of Na<sub>3</sub>MO<sub>4</sub> (M = Np and Pu): The First-Principles Calculations. *Ceramics International*, **46**, 25359-25365. https://doi.org/10.1016/j.ceramint.2020.07.003
- [38] Haines, J., Leger, J.M. and Bocquillon, G. (2001) Synthesis and Design of Superhard Materials. Annual Review of Materials Research, 31, 1-23. <u>https://doi.org/10.1146/annurev.matsci.31.1.1</u>
- [39] Sirdeshmukh, D.B., Sirdeshmukh, L. and Subhadra, K.G. (2011) Atomistic Properties of Solids. Vol. 147, Springer, Berlin, 1-617. <u>https://doi.org/10.1007/978-3-642-19971-4\_1</u>
- [40] Bannikov, V.V., Shein, I.R. and Ivanovskii, A.L. (2007) Electronic Structure, Chemical Bonding and Elastic Properties of the First Thorium-Containing Nitride Perovskite TaThN<sub>3</sub>. *Physica Status Solidi—Rapid Research Letters*, 1, 89-91. <u>https://doi.org/10.1002/pssr.200600116</u>
- [41] Pugh, S. (1954) XCII. Relations between the Elastic Moduli and the Plastic Properties of Polycrystalline Pure Metals. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, **45**, 823-843. https://doi.org/10.1080/14786440808520496
- [42] Duan, J., Zhou, T., Zhang, L., Du, J.-G., Jiang, G. and Wang, H.-B. (2015) Elastic Properties and Electronic Structures of Lanthanide Hexaborides. *Chinese Physics B*, 24, Article ID: 096201. <u>https://doi.org/10.1088/1674-1056/24/9/096201</u>
- [43] Ranganathan, S.I. and Ostoja-Starzewski, M. (2008) Universal Elastic Anisotropy Index. *Physical Review Letters*, **101**, Article ID: 055504. <u>https://doi.org/10.1103/PhysRevLett.101.055504</u>
- [44] Ghosez, P. (1997) First-Principles Study of the Dielectric and Dynamical Properties of Barium Titanate. Doctor Thesis, Universite Catholique de Louvain, Louvain.
- [45] Harrison, W.A. (2012) Electronic Structure and the Properties of Solids: The Phys-

ics of the Chemical Bond. Courier Corporation, Chelmsford.

[46] Granado, E., Moreno, N.O., Garcia, A., Sanjurjo, J.A., Rettori, C., *et al.* (1998) Phonon Raman Scattering in R(1-x)A(x)MnO(3+delta) (R = La, Pr; A = Ca, Sr). *Physical Review B*, **58**, 11435-11440. <u>https://doi.org/10.1103/PhysRevB.58.11435</u>