

## THE FIRST PRINCIPLE STUDY: STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF $X_2ZnN_2$ (X:Ca,Ba,Sr)

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In this work, we used first-principles calculations based on DFT with mBJLDA potential. The properties of tetragonal  $Ca_2ZnN_2$ ,  $Ba_2ZnN_2$  and  $Sr_2ZnN_2$  structures have been investigated using FP-LAPW method. We have calculated the ground-state energy, the lattice constants, density of state (DOS), band gap, optical conductivity and dielectric constant of these structures using Wien2k package. The structure optimization is in good agreement with experimental and theoretical results. All structures present semiconductor band features.  $Ba_2ZnN_2$  and  $Ca_2ZnN_2$  have indirect band gap with 1.345 eV and 1.62 eV values and  $Sr_2ZnN_2$  has direct band gap with 1.45 eV. The calculated optical parameters indicate that all materials are promising candidates for optoelectronic applications.

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**Keywords:** Ab-initio calculations, Wien2k, MBJLDA, Structural properties, Optical properties, Electronic properties

### 1. Introduction

Progress in ternary transition metal nitride research has been important in the last few years [1]. These compounds are quirky and beneficial due to their properties for various applications. [2]. For example, nitride semiconductors are attractive because of environmentally friendly constituents and have useful electronic properties. Specified nitrides having such direct or indirect band structures are well matched to the solar spectrum (band gaps of 0.8 to 1.9 eV). One of these compounds,  $Ca_2ZnN_2$  is especially attractive owing to their earth-abundant elements, low hole and electron effective masses [3].

Theoretical calculations of these structures present semiconductor features. Moreover, some studies reveal the pressure dependence of these compounds. Liang and Zhao (2016) studied first-principles calculations (GGA) of  $Sr_2ZnN_2$  and found 0.775 eV band gap [4]. Matar et al. (2015) looked for crystal and chemical anisotropy effects of  $AE_2Zn_2N_2$  (AE = Ca, Sr, Ba) from first principle calculations [5]. Chern and DiSalvo (1990) synthesized  $Ca_2ZnN_2$  and showed that it was insulating and diamagnetic [6]. Yamane and DiSalvo (1995) synthesized  $Sr_2ZnN_2$  and  $Ba_2ZnN_2$  and determined the structures as tetragonal with space group;  $I 4/mmm$  [7].

It is seen that the electronic and optical properties of these structures are not determined in detail when the present studies are investigated. The compounds  $Ba_2ZnN_2$  and  $Sr_2ZnN_2$  are good candidates for optoelectronic devices and their optical properties have not been investigated. For these reasons, we focus on this study. We studied structural, electronic and optical properties of these compounds and compared the results with previous theoretical and experimental works. In this work, we used the Becke-Johnson potential which is the most successful potential for studying electronic properties of materials [8].

### 2. Computational method

We investigated structural, electronic and optical properties of tetragonal  $Ca_2ZnN_2$ ,  $Ba_2ZnN_2$  and  $Sr_2ZnN_2$  structures within a self-consistent scheme by solving the Kohn-Sham equation based on first principles. For structural optimization, we used PBE (Perdew Burke

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Ernzerhof) potential [9]. To obtain more accurate results, electronic and optical calculations were performed with the modified Becke-Jonhson potential (mBJ) implemented in the Wien2k code [10]. All calculations were performed by using the self-consistent full potential linearized augmented plane wave (FP-LAPW) method [11,12]. In this method, the unit cell is divided into two region that non-overlapping (muffin-tin) spheres and interstitial region. The basis functions are enlarged into spherical harmonic functions inside the muffin-tin sphere (MT) and Fourier series in the interstitial region. The MT sphere radii were selected to be 2.16, 2.40, 2.16, 1.77 and 1.45 a.u. for Ca, Ba, Sr, Zn and N, respectively. The energy of separated the valence and core states was selected as -7 Ry. The convergence of the basis set was checked by a cut off parameter  $R_{mt}K_{max}=8$ , where  $K_{max}$  is the largest mutual lattice vector used in the plane wave dilation and  $R_{mt}$  is the smallest of the MT sphere radii. The magnitude of the largest vector in charge density Fourier expansion ( $G_{max}$ ) was 12. We select the energy convergence criteria as 0.0001 Ry and charge convergence criteria as 0.001e during self-consistency cycles (SCF). In the calculations, we neglected the effect of spin-orbit coupling. The integration over Brillouin zone (BZ) via the tetrahedron method with 159 special k points in the irreducible wedge (2000 k-points in the full BZ) was used to establish the charge density in each self-consistency step. A mesh of  $12 \times 12 \times 12$  has been considered in the whole first Brillouin zone for optical and electronic calculations.

The calculations started with the experimental data and searched for minimum energy depending on volume. The electronic and optical calculations were performed with optimized structure data.

### 3. Results and discussion

#### 3.1. Structural properties

The total energy is determined for various volumes around the experimental cell volume to find the ground state properties of these compounds. The calculated total energies versus volume are fitted to the empirical Murnaghan's equation of state [13] to determine the ground state properties. The calculated total energy as a function of volume  $Ba_2ZnN_2$ ,  $Ca_2ZnN_2$  and  $Sr_2ZnN_2$  are plotted in Fig. 1.

Table 1. Calculated structural parameters of  $X_2ZnN_2$  ( $X:Ca,Ba,Sr$ ).

| Parameter                    | $Ca_2ZnN_2$     | $Ba_2ZnN_2$    | $Sr_2ZnN_2$    |
|------------------------------|-----------------|----------------|----------------|
| $V_0$ (au <sup>3</sup> )     | 549.9663        | 770.046        | 649.8843       |
| $V_{exp}$ (au <sup>3</sup> ) | 548.065 (ref.5) | 761.21 (ref.4) | 649.29 (ref.4) |
| $B_0$ (GPa)                  | 89.33           | 62.09          | 74.43          |
| $B'$ (GPa)                   | 4.05            | 4.43           | 4.34           |
| E (Ry)                       | -6533.146590    | -36368,975639  | -16530.923088  |

According to Murnaghan's equation the calculated volume ( $V_0$ ), bulk modulus ( $B_0$ ), minimum energy (E) and derivative pressure ( $B'$ ) values are listed in Table 1.

The bulk modulus of material shows resistant to compressibility. However, the bulk modulus decreases as the lattice constant increases from  $Ca_2ZnN_2$  to  $Ba_2ZnN_2$  which indicate that these compounds become more compressible and less rigid in that order. Our results are compatible with the well-known relationship [14] between bulk modulus B and the cell volume ( $V_0$ ), as  $B \propto V_0^{-1}$

The calculated cell volume is very close to the experimental results and the deviation value is less than 1.2 % for three compounds.

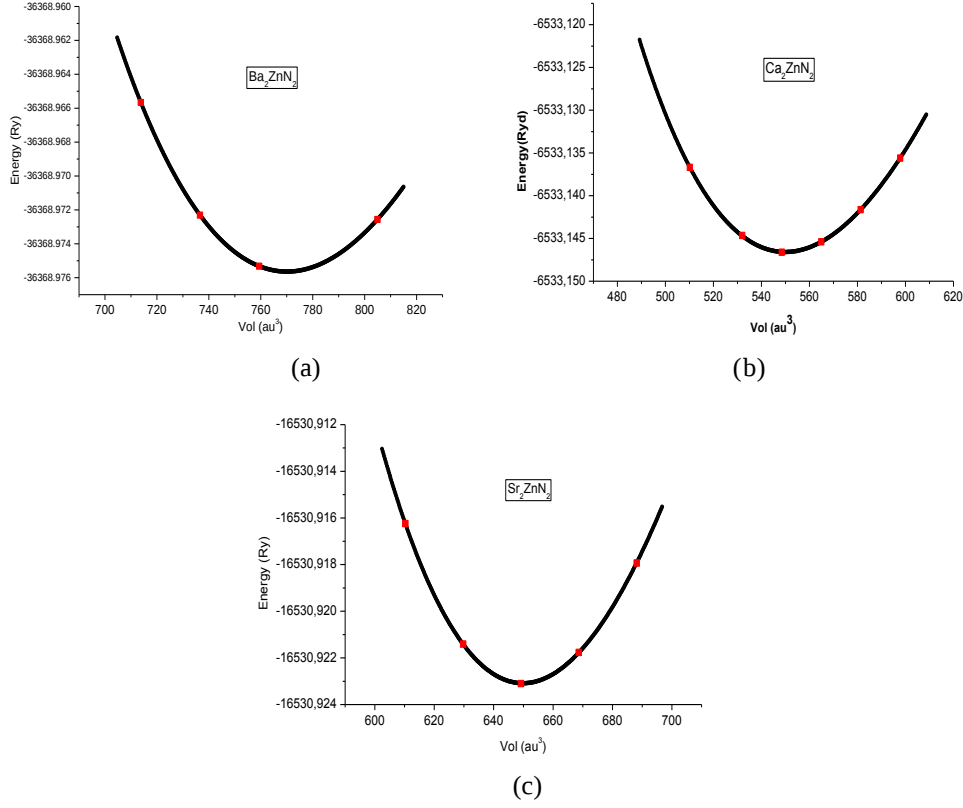


Fig. 1. Total energy of unit cell dependence of unit cell volume  
(a)  $\text{Ba}_2\text{ZnN}_2$  (b)  $\text{Ca}_2\text{ZnN}_2$  (c)  $\text{Sr}_2\text{ZnN}_2$ .

The structural stability of cell is verified by cohesive energy calculation. According to cohesive energy;

$$E_{coh} = E_{X_2ZnN_2}^{tot} - kE_X^{tot} - mE_{Zn}^{tot} - nE_N^{tot}$$

where  $E_{X_2ZnN_2}^{tot}$ ,  $E_X^{tot}$ ,  $E_{Zn}^{tot}$ ,  $E_N^{tot}$  are total energy for  $X_2\text{ZnN}_2$  unit cell, isolated X (Ba,Ca,Sr), Zn and N atoms, respectively. k, m and n indexes are indicator to the number of each atom in the cell.

We obtained the value of cohesive energy -4.59, -5.03, and -3.25 eV/atom for  $\text{Ba}_2\text{ZnN}_2$ ,  $\text{Ca}_2\text{ZnN}_2$  and  $\text{Sr}_2\text{ZnN}_2$ , respectively. Cohesive energy results reveal that the compounds have good stability.

### 3.2. Electronic properties

It is well known that the density of states (DOS) and electronic band structure are important quantities to determine the crystal structure [15]. In order to find bonding character clearly, the total and partial DOS are calculated, as shown in Fig. 2. In the Fig. 2, the Fermi energy was set at the zero point.

Total DOS curve of  $\text{Ba}_2\text{ZnN}_2$  mainly divided into four parts (Fig.2.a). The valence band nearly Fermi level is essentially dominated by N-p states and minor presence of Zn-p and Zn:d states. The intermediate valence band (nearly -7 eV) is essentially dominated by Zn:d states. The core band (between 11 eV and 13 eV) is dominated by Ba:p states. The most contribution on conduction band comes from Ba:d and N:p states (Fig. 2b). The valence band and conduction band separated by band gap nearly 1.4 eV.

The total DOS of  $\text{Ca}_2\text{ZnN}_2$  has three divided parts (Fig. 2c). The intermediate valence band (around -7 eV) is essentially dominated by Zn:d orbital. The valence band from -4 eV to Fermi level is essentially dominated by N:p states and there are less contribution from Zn:d, Zn:p and Ba:d states. At the conduction band most contribution comes from Ca:d and minor contribution from N:p states (Fig. 2d). The valence band and conduction band are separated by 1.6 eV band gap.

Total DOS of  $\text{Sr}_2\text{ZnN}_2$  is consisting of four divided parts (Fig. 2e). Around -12 eV the core electron dominated by Sr:d states. Valence band around -7 eV essentially dominated by Zn:d electrons. Valence band nearly Fermi level is essentially dominated by N:p states and minor presence of Zn:d, Zn:p and Sr:d states. The conduction band from 0 eV and 4 eV is dominated by N:p and Sr:d states.

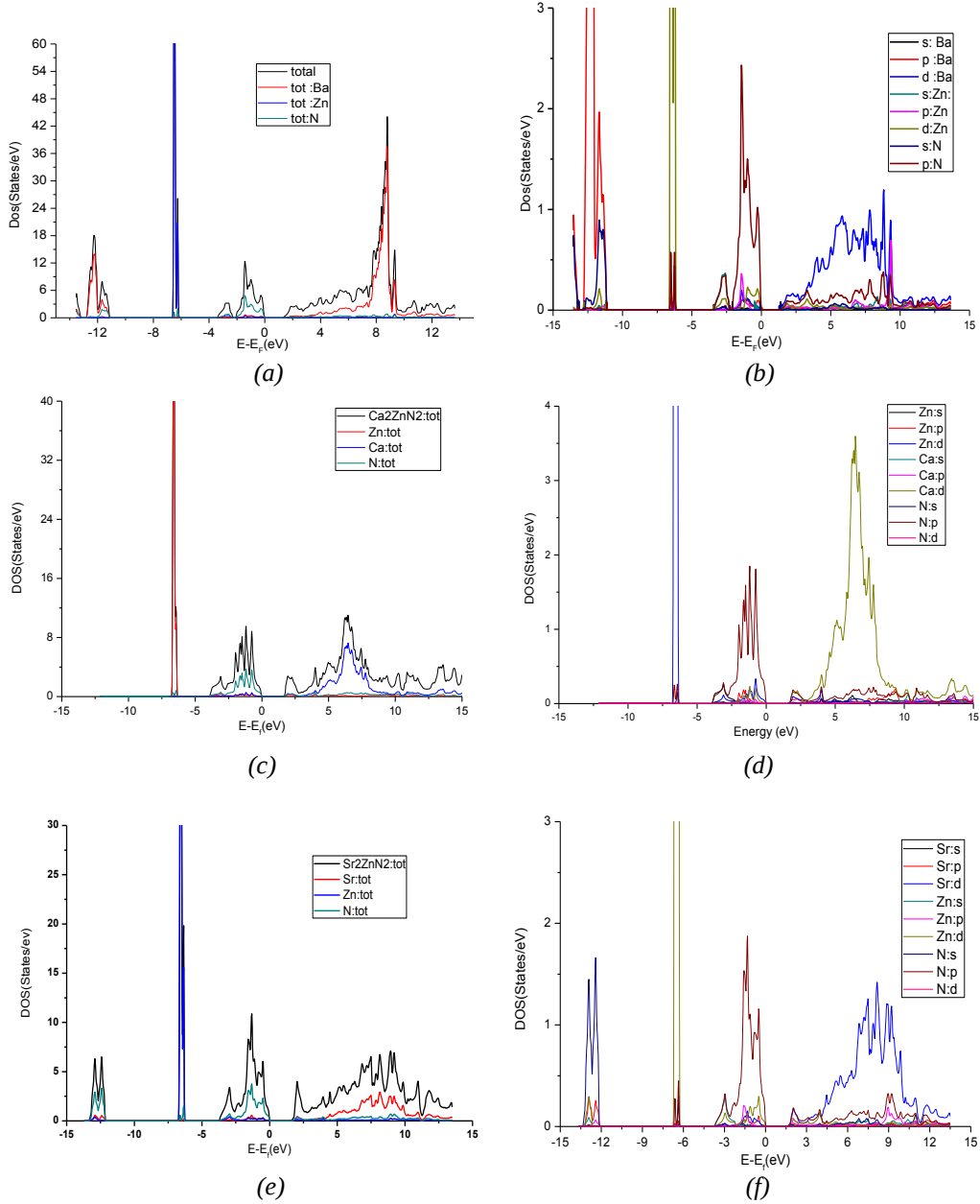


Fig. 2. Calculated total and partial DOS (a) total DOS of  $\text{Ba}_2\text{ZnN}_2$ , (b) partial DOS of  $\text{Ba}_2\text{ZnN}_2$ , (c) total DOS of  $\text{Ca}_2\text{ZnN}_2$ , (d) partial DOS of  $\text{Ca}_2\text{ZnN}_2$ , (e) total DOS of  $\text{Sr}_2\text{ZnN}_2$  and (f) partial DOS of  $\text{Sr}_2\text{ZnN}_2$ .

The conduction band from 4 eV to 15 eV is essentially dominated by Sr:d states. The valence band and conduction band are separated by 1.4 eV band gap (Fig. 2f). Evidently, the total DOS of  $\text{Ba}_2\text{ZnN}_2$ ,  $\text{Ca}_2\text{ZnN}_2$  and  $\text{Sr}_2\text{ZnN}_2$  exhibit semiconductor feature.

We plotted the electronic band chart to understand the electronic properties of the structures. In the Fig. 3, the Fermi level is set as zero energy level. As seen from Fig. 3a, top of valence band is located at the high symmetry point  $\Gamma$  while the bottom of conduction band is located at the M in the first Brillouin Zone (BZ) [16]. Ba:3d states mainly constitute of conduction band minimum and N:2p constitute valence band maximum (Fig. 2.b). Therefore  $\text{Ba}_2\text{ZnN}_2$  has an indirect band gap with value of 1.345 eV.

It can be seen from Fig. 3b, the valence band maximum (VBM) is located at the high symmetry point Z and the conduction band minimum (CBM) is located at the  $\Gamma$  in the Brillouin Zone. Valence band maximum mainly consist of N:2p states and conduction band minimum consist of Ca:3d and N:2p states (Fig. 2d). So that,  $\text{Ca}_2\text{ZnN}_2$  has an indirect band gap with value of 1,62 eV.

Electronic band plots of  $\text{Sr}_2\text{ZnN}_2$  (Fig. 3c) shows that, top VBM is located at the high symmetry point  $\Gamma$  and the CBM is located at the  $\Gamma$  point in the Brillouin Zone. Valence band maximum mainly consist of N:2p states and conduction band minimum consist of N:2p states (Fig. 2f.). So that,  $\text{Sr}_2\text{ZnN}_2$  has a direct band gap with value of 1.45 eV

Table 2. Theoretical and experimental band gap values of  $\text{Ba}_2\text{ZnN}_2$ ,  $\text{Ca}_2\text{ZnN}_2$  and  $\text{Sr}_2\text{ZnN}_2$ .

| Parameter                 | Direct band gap (eV)                                         | Indirect band gap (eV)                                      |
|---------------------------|--------------------------------------------------------------|-------------------------------------------------------------|
| $\text{Ba}_2\text{ZnN}_2$ | 1,42 <sup>a</sup> 1,40 <sup>c</sup>                          | <b>1,35</b> <sup>a</sup> 1,3 <sup>c</sup>                   |
| $\text{Ca}_2\text{ZnN}_2$ | 1,72 <sup>a</sup> 1,9 <sup>b</sup> 1,92 <sup>c</sup>         | <b>1,62</b> <sup>a</sup> 1,6 <sup>b</sup> 1,65 <sup>c</sup> |
| $\text{Sr}_2\text{ZnN}_2$ | <b>1,45</b> <sup>a</sup> 1,7 <sup>c</sup> 0,775 <sup>d</sup> | 1,9 <sup>a</sup>                                            |

<sup>a</sup> This work <sup>b</sup> Experimental values ref.2. <sup>c</sup> Theoretical values ref.2. <sup>d</sup> Theoretical values ref.3.

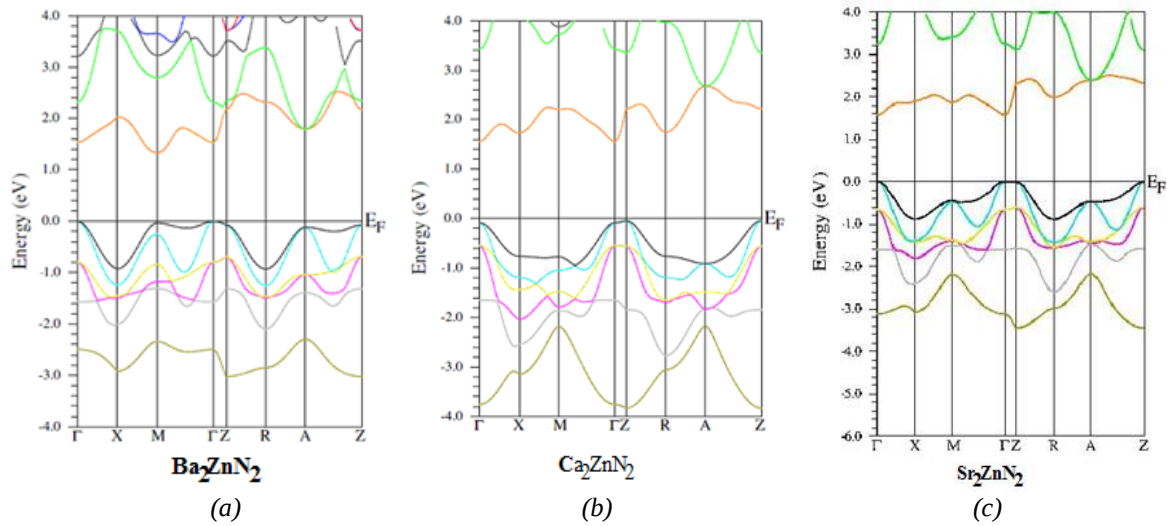


Fig. 3. Calculated band plot of (a)  $\text{Ba}_2\text{ZnN}_2$ , (b)  $\text{Ca}_2\text{ZnN}_2$  (c)  $\text{Sr}_2\text{ZnN}_2$ .

### 3.3. Optical properties

It can be possible to suggest potentially new optoelectronic applications by studying optical properties of materials [17]. Thus, we calculated dielectric function, optical conductivity, absorption and reflection of  $\text{Ba}_2\text{ZnN}_2$ ,  $\text{Ca}_2\text{ZnN}_2$  and  $\text{Sr}_2\text{ZnN}_2$  to contribute this area.

### 3.3.1. Dielectric function

One of the best approaches to investigate the optical properties of materials can be considered as calculation of the complex dielectric function [18]. The optical response of a medium at all photon energies is described by the dielectric function:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

The real part  $\varepsilon_1(\omega)$  is related to the dispersive conduct and the imaginary part  $\varepsilon_2(\omega)$  corresponds to the absorptive conduct of the material. The other optical properties can be directly calculated from  $\varepsilon_1(\omega)$  and  $\varepsilon_2(\omega)$  [19]. The calculated real and imaginary parts of the dielectric function for  $\text{Ba}_2\text{ZnN}_2$  is plotted in Fig. 4.

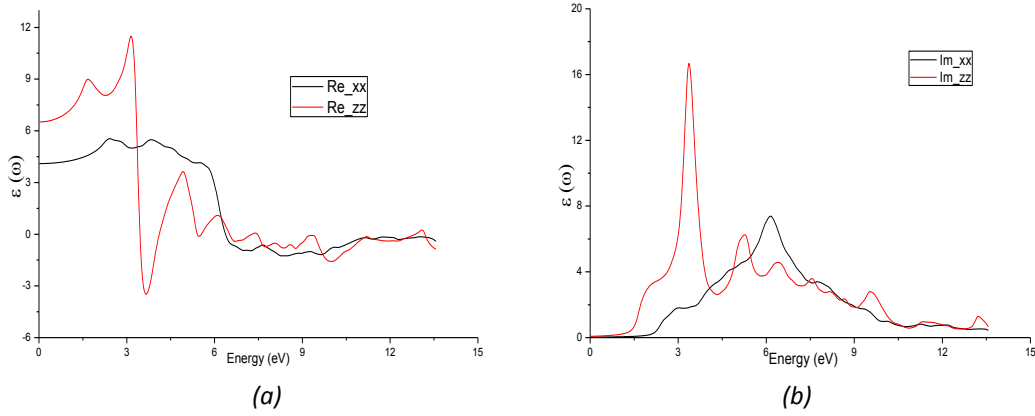


Fig. 4. Calculated real and imaginary part of epsilon for  $\text{Ba}_2\text{ZnN}_2$  with xx and zz directions  
(a) real part of epsilon b) imaginary part of epsilon.

As it can be seen in the Fig. 4a, the static values ( $\varepsilon_0$ ) of the real part of dielectric constant in xx direction is  $\varepsilon_0 = 4.1$  and in the zz direction is  $\varepsilon_0 = 6.5$ . The maximum value of the real part dielectric constant is 5.5 in xx direction and 11.5 in zz direction. The minimum value of the real part dielectric constant is -1.26 in xx direction and -3.5 in zz direction. The imaginary parts of dielectric coefficient edge are 1.2 eV for xx and 2 eV for zz direction. Optical spectra exhibit anisotropy in two directions (along basal-plane and z-axis).

The calculated real and imaginary part of the dielectric function of  $\text{Ca}_2\text{ZnN}_2$  compound is plotted in Fig. 5.

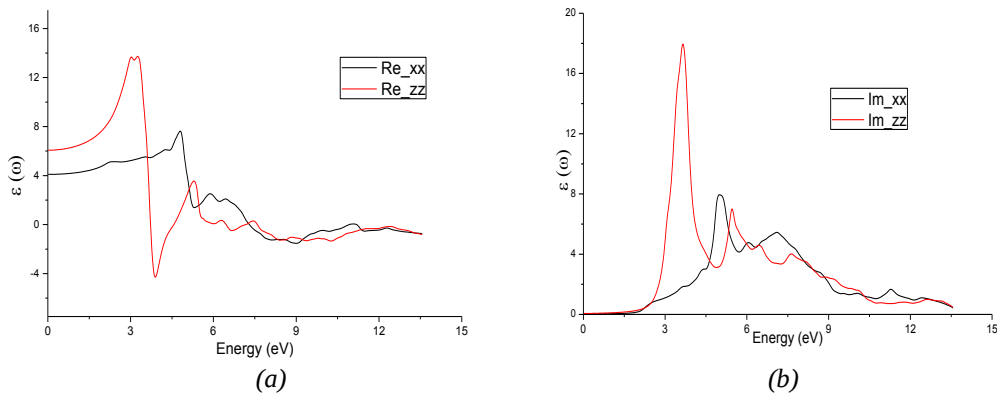


Fig. 5. Calculated real and imaginary part of epsilon for  $\text{Ca}_2\text{ZnN}_2$  with xx and zz directions  
(a) real part epsilon b) imaginary part of epsilon.

As it can be seen in Fig. 5a the static dielectric constant ( $\epsilon_0$ ) of real part in xx direction is  $\epsilon_0=4.1$  and  $\epsilon_0=6.1$  in the zz direction. The real parts of dielectric constant have the maximum value as 7.6 in xx and 13.7 in zz direction. The minimum value of the real part dielectric constant is -1.5 in xx and -4.2 in zz direction. The imaginary parts of the dielectric coefficient edge are nearly 1.5 eV for xx direction and 2 eV for zz direction. Optical spectra show anisotropy in two directions.

The calculated real and imaginary parts of the dielectric function of  $\text{Sr}_2\text{ZnN}_2$  are plotted versus photon energy as depicted in Fig. 6. As seen in the Fig. 6a; the static values of real part of dielectric constant ( $\epsilon_0$ ) in xx is  $\epsilon_0=4.1$  and in the zz direction is  $\epsilon_0=6.07$ . The maximum value of the real part dielectric constant is 7.63 in xx and 13.73 in zz direction.

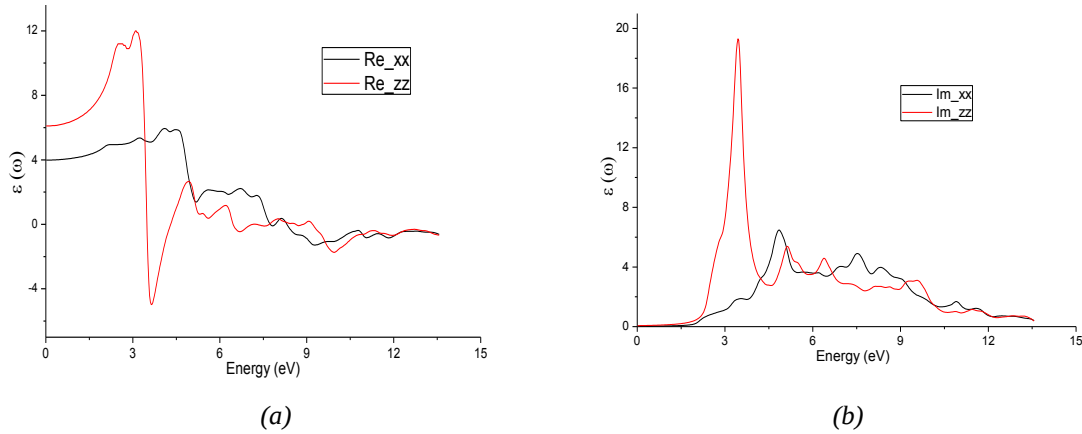


Fig. 6. Calculated real and imaginary part of epsilon of  $\text{Sr}_2\text{ZnN}_2$  with xx and zz directions  
(a) real part of epsilon b) imaginary part of epsilon.

The minimum value of the real part dielectric constant is -1.53 in xx and -4.28 in zz direction. The imaginary part of the dielectric coefficient edge is 1.7 eV for xx and 2 eV for zz direction. Optical spectra show anisotropy in two directions.

### 3.3.2. Absorption coefficient

The absorption coefficient indicates the ability of a material to absorb the incident photon of specific energy [18]. It is given as follows:

$$\alpha(\omega)_j = 2\omega / c(-\text{Re}(\epsilon(\omega)_j) + |\epsilon(\omega)_j|/2)^{1/2}$$

The calculated absorption coefficients of  $\text{Ba}_2\text{ZnN}_2$ ,  $\text{Ca}_2\text{ZnN}_2$  and  $\text{Sr}_2\text{ZnN}_2$  are plotted in Fig. 7. The absorption part of  $\text{Ba}_2\text{ZnN}_2$  spectra starts at 1.4 eV in xx, and 2 eV energy in zz direction as can be seen in Fig. 7a. As shown in Fig. 7b; the absorption part of  $\text{Ca}_2\text{ZnN}_2$  spectra starts at 1.9 eV in xx, and 1.9 eV energy in zz direction which 0.8 eV above the indirect band gap.

As can be seen in Fig. 7c; the absorption part of  $\text{Sr}_2\text{ZnN}_2$  spectra starts at 1.95 eV in xx and 1.95 eV energy in zz direction which is 0.5 eV above the direct band gap.

The value of absorption coefficient rapidly increases when the incident photon energy became higher than the absorption edge. On the other hand, the absorption coefficients rapidly decrease in the high energy region and this is a typical characteristic of semiconductors.

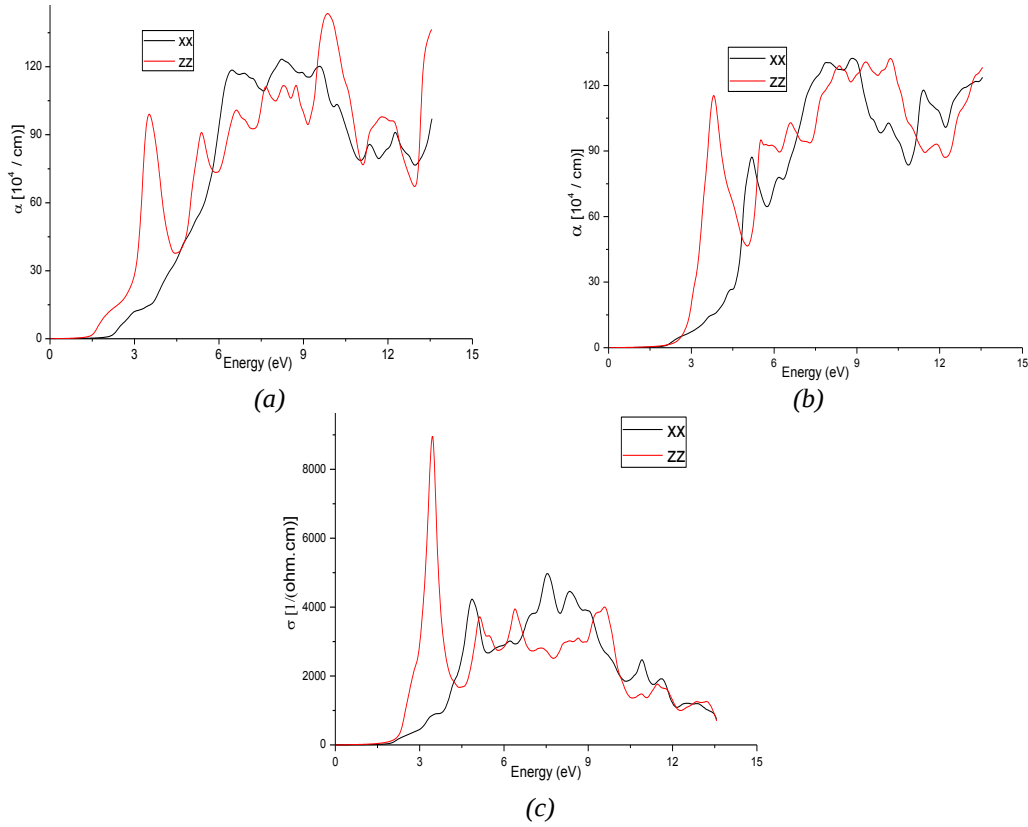


Fig. 7. Calculated optical absorption for xx and zz directions  
(a)  $Ba_2ZnN_2$ , (b)  $Ca_2ZnN_2$ , (c)  $Sr_2ZnN_2$

### 3.3.3. Optical conductivity

The optical conductivity corresponds to the conduction of electrons produced when a photon of a certain frequency is incident upon a material [18]. The optical conductivities of  $Ba_2ZnN_2$ ,  $Ca_2ZnN_2$ , and  $Sr_2ZnN_2$  are given in Fig. 8.  $E_0$  is initial energy of absorption. In the calculated  $E_0$ , the first two peaks and the maximum value of sigma for  $Ba_2ZnN_2$ ,  $Ca_2ZnN_2$  and  $Sr_2ZnN_2$  are given in Table 3. It can be seen from Fig. 8,  $Ca_2ZnN_2$ ,  $Ba_2ZnN_2$  and  $Sr_2ZnN_2$  compounds have high optical conductivity in the visible light region (1.65–3.1 eV). This is important for solar cell materials.

Table 3. Optical conductivity (sigma) parameters of  $Ba_2ZnN_2$ ,  $Ca_2ZnN_2$  and  $Sr_2ZnN_2$ .

| Parameter-Direction |    | $E_0$ (eV) | $E_1$ (eV) | $E_2$ (eV) | $\sigma_{max}$ [1 / (Ohm cm)] |
|---------------------|----|------------|------------|------------|-------------------------------|
| $Ba_2ZnN_2$         | xx | 1,3        | 6,16       | 7,8        | 6119                          |
|                     | zz | 2          | 3,38       | 5,29       | 7561                          |
| $Ca_2ZnN_2$         | xx | 1.5        | 5,07       | 6,11       | 5380                          |
|                     | zz | 2          | 3,66       | 5,5        | 8841                          |
| $Sr_2ZnN_2$         | xx | 1.5        | 4,86       | 7,5        | 4970                          |
|                     | zz | 2          | 3,44       | 5,1        | 8950                          |

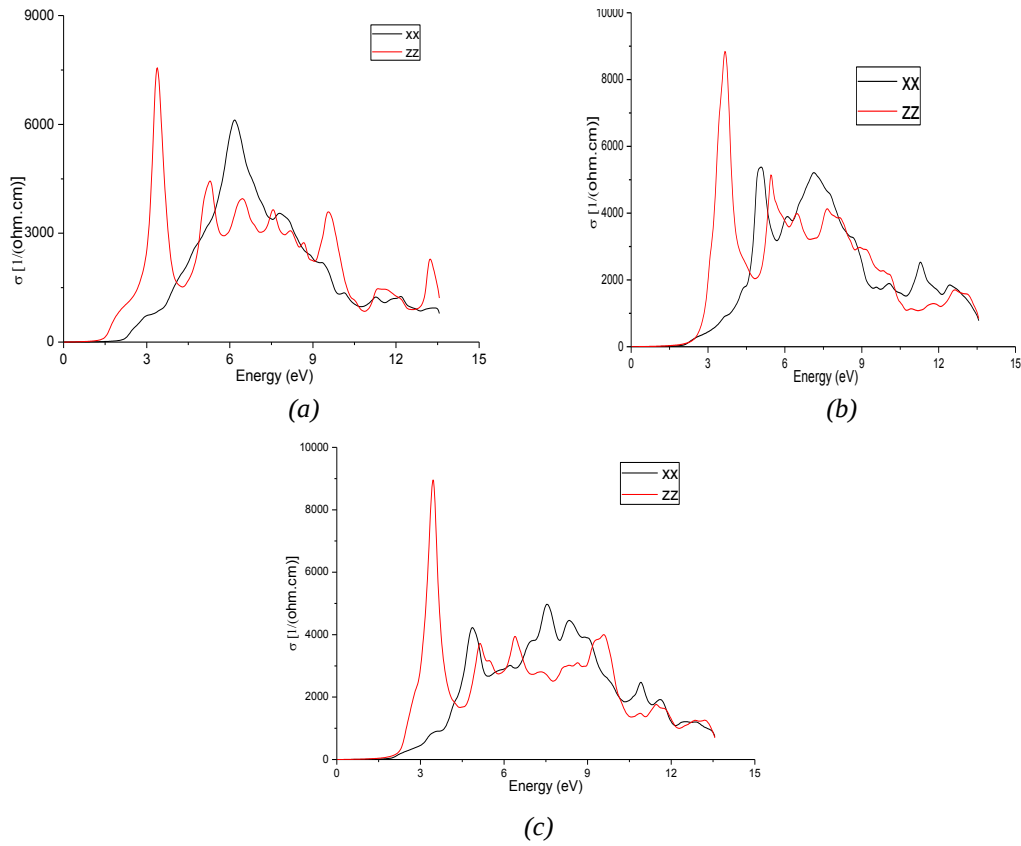


Fig. 8. Calculated optical conductivity of (a)  $\text{Ba}_2\text{ZnN}_2$ , (b)  $\text{Ca}_2\text{ZnN}_2$ , (c)  $\text{Sr}_2\text{ZnN}_2$ .

#### 4. Conclusions

We have explored structural, electronic and optical properties of  $\text{Ba}_2\text{ZnN}_2$ ,  $\text{Ca}_2\text{ZnN}_2$  and  $\text{Sr}_2\text{ZnN}_2$  employing all electrons full potential linearized augmented plane wave (FP-LAPW) method based on DFT within modified Becke-Jonhson potential (mBJ). The calculated cell constants are compatible with experimental works. The calculated electronic band structure shows that all structures reveal semiconductor band character for  $\text{Ba}_2\text{ZnN}_2$  and  $\text{Ca}_2\text{ZnN}_2$  having indirect band gap with 1.345 and 1.62 eV values, respectively.  $\text{Sr}_2\text{ZnN}_2$  has direct band gap with 1.45 eV. Optical nature of  $\text{Ba}_2\text{ZnN}_2$ ,  $\text{Ca}_2\text{ZnN}_2$ , and  $\text{Sr}_2\text{ZnN}_2$  is explored with the help of calculating optical parameters such as absorption coefficient, dielectric function, and optical conductivity for photon energy up to 14.0 eV. The optical features of these compounds show anisotropy in xx and zz directions.

The calculated electronic and optical parameters show that all compounds are good candidates for optoelectronic applications.

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