



Tuning of electronic and optical properties in ZnX (X=O, S, Se and Te) monolayer: Hybrid functional calculations

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ABSTRACT

The structural, electronic and optical properties of graphene-like ZnX (X=O, S, Se and Te) are investigated in the framework of the density functional theory. Calculating strain energy exhibits that all compound has an asymmetric behavior with respect to applied biaxial strain. The electronic results indicate that the electronic properties of the considered layered compounds such as energy gap and gap direction can be tuned using exerting biaxial in-plane compressive and tensile strains. It has been shown that both compressive and tensile strains decrease the energy gap of ZnO monolayer. However, for the other compounds, ZnS, ZnSe and ZnTe, the energy gap increases by applying compressive strain while it decreases under tensile strains, respectively. The band gap direction changes by imposing different types strains. The optical results exhibit red shift and blue shift in the optical absorption spectrum for ZnO and ZnS monolayers by exerting tensile and compressive strains, respectively. Our obtained results suggest that these wide gap semiconductors can be good candidate for optoelectronic nano-base device.

1. Introduction

In the last decade, two-dimensional nanostructures could find a unique location in nanotechnology applications and devices. Because of their unique properties such as high surface area, good synthesis conditions, controlling on their properties, etc., they can be used in many industrial fields for example energy storage [1], electronic [2], biomedicine [3] and sensors [4]. Some unexpected properties of graphene [5] have made a lot research groups to put our interest in predicting and studying the other two-dimensional materials such as h-BN [6-8], transition metal chalcogenides [9,10], alkali halides [11,12], metallic oxides [13-15], phosphorene [16], silicone [17] and other types of two dimensional nano materials [18-21]. Among these categories, zinc oxide and zinc chalcogenides are so favorable semiconductor for electronic and optical applications. ZnO and ZnS have attracted attention owing to their many applications specially in nano-electronic and nano-photoelectric such as photoluminescence, photo catalysis, light-emitting

diodes (LEDs), field effect transistors (FET), sensors, dye-sensitized solar cells and field emission (FE) [2,3,10]. Peng *et al.* investigated mechanical properties of graphene-like hexagonal zinc oxide monolayer (g-ZnO) using first-principles calculations based on density-functional theory. They proposed that compared to hexagonal boron nitride monolayer (g-BN), g-ZnO much softer they also proposed that g-ZnO has a larger Poisson's ratio. They showed that second order elastic constants increase with pressure while the Poisson's ratio decreases with increasing pressure [22-24]. Exerting stress and strain on these types of nanomaterials is one of the best strategies for controlling and tuning electronic and optical properties if them. In some previous work, we showed that some two-dimensional materials such as BN [25], InN [26], BeS [27] and Be₂C [28] can be tuned by applying biaxial stress and strain. The results express that electronic properties of these semiconductor nanostructures such as energy gap and gap direction can be controlled by different values of strain on system, also optical properties such as absorption and optical conductivity of

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them are so sensitive to structural deformation too.

In our previous work, we studied the electronic and optical properties of ZnX and CdX (X=S, Se and Te) graphene-like monolayers¹⁰. The results illustrated that the threshold of absorption spectrum shifts toward higher energies from S to Te atoms. So, in this article, the electronic properties of ZnX (X=O, S, Se and Te) graphene-like monolayers are studied under different biaxial stress and strain condition to gain a controllability of electronic properties.

2. Computational Method

Using first principles calculations, the electronic properties of ZnX (X=O, S, Se and Te) monolayer are tuned by exerting different biaxial compressive and tensile strains conditions. Full potential linear augmented plane waves plus local orbital's (FP-LAPW+lo) are used to expand Kohn-Sham wave functions [29]. WIEN2k code is utilized to perform all calculations such as optimization, structural and electronic [30]. All input parameters were optimized to gain an acceptable accuracy in presenting results. Optimized $R_{\text{MT}}K_{\text{max}}$ used 8, and the charge density, was expanded to $G_{\text{max}}=14 \text{ Ry}^{1/2}$. Since the generalized gradient approximation (GGA) method tends to underestimate the band gap, we also computed and compared the results using GGA presented by Perdew-Burke-Ernzerhof [31] and screened hybrid functional, HSE06 [32]. using Monkhorst-Pack scheme a $30 \times 30 \times 1$ and $48 \times 48 \times 1$ k -meshes are used to expand k -point in the first Brillouin zone [33] for electronic and optical calculations, respectively. Also, Vacuum layers with a minimum thickness of 20 angstrom in the non-periodic directions (z -axis) were utilized in our calculations to avoiding adjacent monolayer interaction.

3. Results and Discussion

3.1. Structural Calculations

In this section the structural properties and the stability of ZnX (X=O, S, Se and Te) monolayers under stress and strain conditions are investigated. As the first step, using thermodynamic equation state of Brich-Murnaghan [34], lattice constants are optimized. The obtained optimized values are in a good agreement with previous works [10,35,36]. To investigate the effects of strain or stress, all atoms are allowed to be fully free to move within their planes. Furthermore, the quasi-Newton scheme is used to relaxation process of all atoms into equilibrium positions within the deformed unit cell that results the minimum total energy for the imposed strain and stress states of the unit cell. The variations of the lattice constants in different stress and strain conditions are considered as follows:

$$a_{\pm\delta} = a_{eq}(1 \pm \delta) \quad (1)$$

where $\delta = 2\%$; 4% ; 6% and 8% , a_{eq} is the equilibrium lattice constant (free-strained case). $a_{-\delta}$ and $a_{+\delta}$ are

denote to compressive and tensile lattice parameters, respectively. In this definition and the positive and negative signs refer to strained and stressed systems, respectively. The strain energy per atom is defined as:

$$E_s(\delta) = (E_{tot}(\delta) - E_{free})/n \quad (2)$$

where $E_{tot}(\delta)$, E_{free} and n are the total energy of system, total energy of free-strained system and the number of atoms in considered unit cell, respectively. The obtained strain energy versus applied different biaxial strain is illustrated in the figure 1 for all compounds. We can see a different behavior for strain energy in tensile and compression conditions, so there is an asymmetrical variation in strain energy. This asymmetry illustrates the elastic disharmony of the ZnX (X=O, S, Se and Te) two-dimensional structures which can be referred to bond nature of compounds. One can see that among the considered compounds ZnTe has the lowest elastic symmetry (see Fig. 1a).

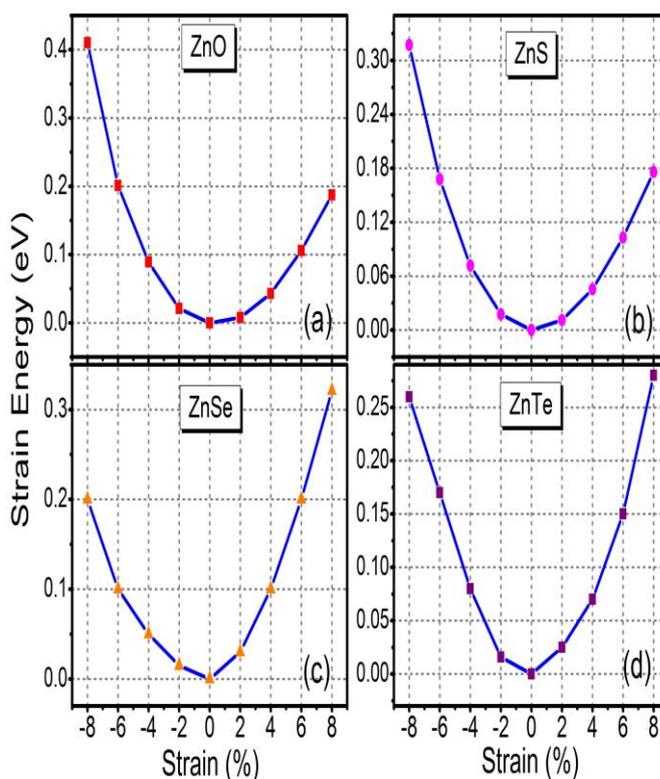


Figure 1. Calculated strain energy versus applied biaxial strain for (a) ZnO, (b) ZnS, (c) ZnSe and (d) ZnTe.

3.2. Electronic Properties

Studying electronic and optical properties of semiconductor materials is so sensitive to energy gap values of them. There are different exchange-correlation terms to calculate gap value of materials with high accuracy. Here, GGA-PBE and screened hybrid functional, HSE06, are used to calculate electronic properties of compounds in free-strained cases. The results illustrate that the energy gap values of HSE06

functional are larger than GGA-PBE results. All obtained values are summarized in Tab. 1. So, all calculations for strained systems will be done with HSE06 approach.

Table 3. Calculated energy gap (eV) for free-strained cases of compounds using both GGA-PBE and HSE06 functionals.

	GGA-PBE	HSE06
ZnO	1.673	3.175
ZnS	2.521	3.712
ZnSe	0.609	1.656
ZnTe	0.169	1.087

Needless to say, to control energy band gap of the semiconductors is essential in electronic and optical applications. For the aim of energy band gap engineering, different methods such as imposing stress and strain, doping, and applying an electric field are used. In this research, the effect of biaxial strain and stress on the energy band gap of ZnX (X=O, S, Se and Te) graphene-like monolayers is investigated, where, the FPLAPW+lo method is used. As the first case, the zinc oxide monolayer is studied (see figure 2). As seen in figure 2, by applying stress and strain on ZnO monolayer its energy band gap is reduced.

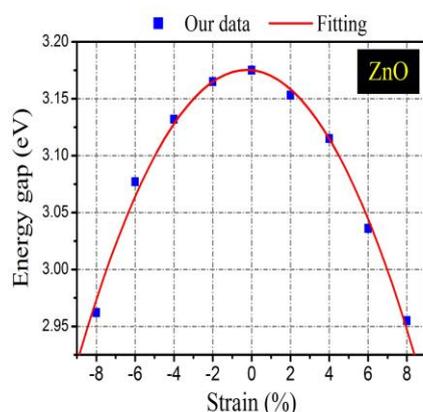


Figure 2. Calculated energy gap of ZnO versus strain. The blue cubes are our data and red line is fitted curve.

To more investigate, the energy band gap of the monolayer under different stress and strain conditions is calculated. To gain a deeper insight on the behavior of the in our study, when strain or stress are applied to the monolayer compound, all atoms are allowed to be fully free to move within their planes. Furthermore, the quasi-Newton scheme is used to relaxation process of all atoms into equilibrium positions within the deformed unit cell that results the minimum total energy for the imposed strain and stress states of the unit cell. To gain more accurate prediction of the behavior of the ZnO monolayer under stress and strain condition, using the obtained energy band gap values, a fitting process was

done, where, the order of the energy band gap equation was increased to a second degree polynomial:

$$E_{gap}^{ZnO} = A + B_1x + B_2x^2 \quad (3)$$

where the values of $A=3.1751$, $B_1=-0.0016$ and $B_2=0.0033$ were calculated. To estimate the accuracy of the fitting process a regression coefficient R^2 was calculated, where the value of $R^2=0.992$ was obtained which confirms a very good accuracy of the process. As seen in Fig. 2, by applying compressive and tensile strains the energy band gap of the ZnO monolayer is slightly reduced. As about 13.5% gap reduction with respect to free-strained case is occurred not only for the maximum value of considered biaxial stress but also for the maximum value of considered biaxial stress condition. This behavior is due to the nature Zn-O bonds. The Zn-O bond has almost a strong ionic nature because of the difference between the electronegativity of Zinc and Oxygen atoms, which is 1.65 for Zinc and 3.44 for oxygen atoms in Pauling's scale. By applying biaxial compressive and tensile strains, the strength of the planar σ bonds are decreased, so the energy difference between valence and conduction bands decreases. Now, let us investigate the zinc sulphide monolayer. The electronic and magnetic properties of ZnS monolayer have been studied by some computational groups. According to the fitting process, the band gap versus strain values can be represented by a second order equation:

$$E_{gap}^{Zns} = A + B_1x + B_2x^2 \quad (4)$$

where $A=3.465$, $B_1=-0.12131$ and $B_2=-0.0035$, where the obtained value of 0.999 for the regression coefficient R^2 denotes a good fitting process. By applying stress, the Zn-S bond length is reduced, so that a strong sigma bond in x - y plane (sp^2 bonds) is occurred, i.e., the energy band gap is increased, where, the band gap increasing of about 25% is occurred in 8% compress with respect to free-strained case (see Fig. 3). However, for tensile strain condition, the band gap reduction of about 35% is seen for 8% strained case with respect to free-strained system.

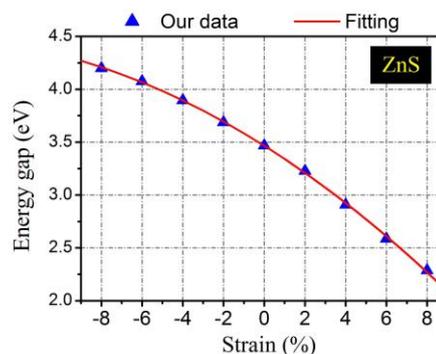


Figure 3. Calculated energy gap of ZnS versus strain. The blue cubes are our data and red line is fitted curve.

In continue, the energy band gap variations of ZnSe and ZnTe compounds are studied. The behavior of the energy band gap of ZnSe monolayer is similar to ZnS (see Fig. 4). Furthermore, using the fitting process, the order of the energy band gap equation was increased to a second degree polynomial:

$$E_{gap}^{ZnSe} = A + B_1x + B_2x^2 \quad (5)$$

where $A=1.654$, $B_1=-0.13888$ and $B_2= 0.00292$, and the obtained value of 1 for the regression coefficient indicates a high accuracy of the fitting process. Finally, as seen in figure 5, similar to ZnSe, the energy band gap of ZnTe compound moves towards zero by applying biaxial tensile strain up to higher percent of strain. One may claim that this general trend from ZnS to ZnTe, vanishing energy gap, maybe its related to anionic radii that effects on ionic-covalent behavior of bonds. As by increasing in anion atom radii's, the energy gap moves toward zero value in lower strain ranges. The obtained gap variation function for ZnTe compound presented below:

$$E_{gap}^{ZnTe} = A + B_1x + B_2x^2 \quad (6)$$

where $A=1.097$, $B_1= -0.12905$ and $B_2=0.00481$, and square regression coefficient is $R^2=1$. Therefore, we can see a tuning of energy band gap in considered monolayer by applying stress and strain. These results can help us to design new two-dimensional nanomaterial based devices in electronic and optic industries.

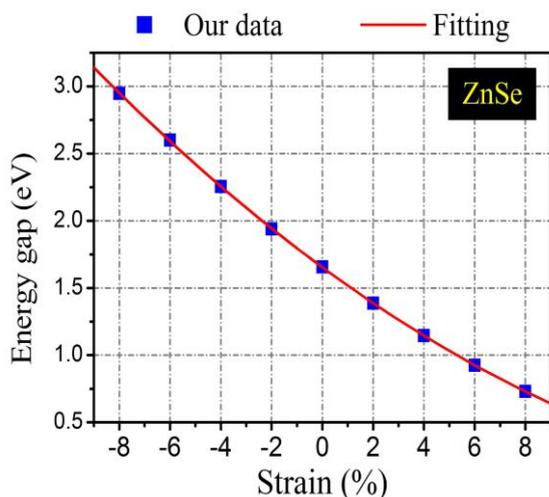


Figure 4. Calculated energy gap of ZnSe versus strain. The blue cubes are our data and red line is fitted curve.

To more investigation in the electronic properties of the considered materials, the electronic band structure of all compounds under different stress and strain conditions is studied. A schematic of the bond interactions in both compressive and tensile strain conditions are shown in Fig. 6. Needless to say that due to the occupation states of bonding $px+py$ and non-bonding p_z orbitals of each atom in these compounds, different bond interactions are exhibited by the monolayers.

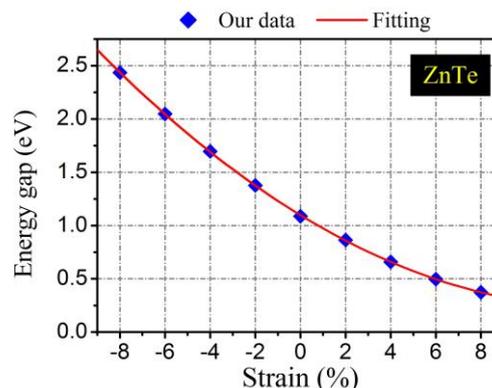


Figure 5. Calculated energy gap of ZnTe versus strain. The blue cubes are our data and red line is fitted curve.

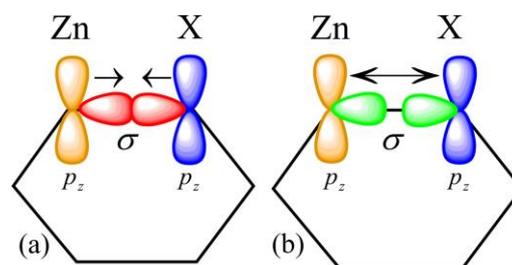


Figure 6. Schematic presentation of orbital situations in (a) compress and (b) tensile strain conditions.

The energy band structure of ZnO monolayer under different compressive and tensile strain conditions are illustrated in the figure 7. As seen in figure 7, the ZnO monolayer is a direct gap semiconductor ($\Gamma \rightarrow \Gamma$), and it is remained a direct band gap semiconductor in the whole considered stress and strain ranges. Band structure analysis demonstrates that the valence band maximum (VBM) belongs to $px+py$ orbitals of oxygen atoms while the conduction band minimum (CBM) refers to p_z unoccupied states of zinc atoms. Although the gap direction remains Γ to Γ , the exerting of strain causes to arising the energy level in K direction with respect to Γ direction. The energy level in K direction for valence band is composed by p_z orbitals of oxygen atoms. One may claim by applying tensile strain to the monolayer the $px+py$ bonds become weak, so the energy of these orbitals changes with respect to p_z orbitals.

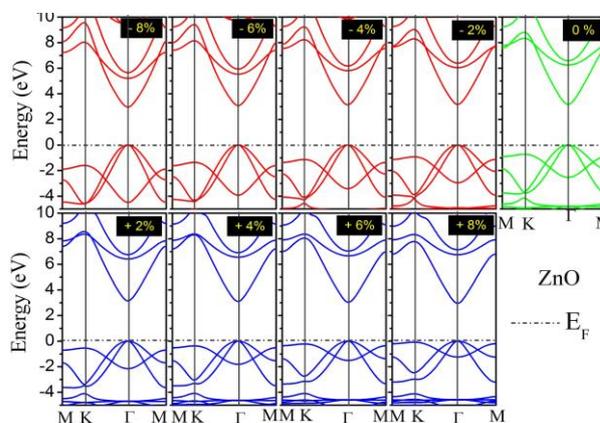


Figure 7. Calculated energy band structure of ZnO monolayer for all values of considered strain.

As seen in figure 8, the ZnS monolayer exhibits a direct energy band gap of about 3.7 eV in Γ direction. Different from ZnO monolayer, for the ZnS monolayer, by applying biaxial tensile strain a displacement of energy levels changes the VBM point, so the energy band gap becomes indirect ($K \rightarrow \Gamma$). However, for the compressed system, the energy level in K point moves towards lower energies with respect to bonding $px+py$ orbitals in Γ direction, so that the energy band gap remains direct.

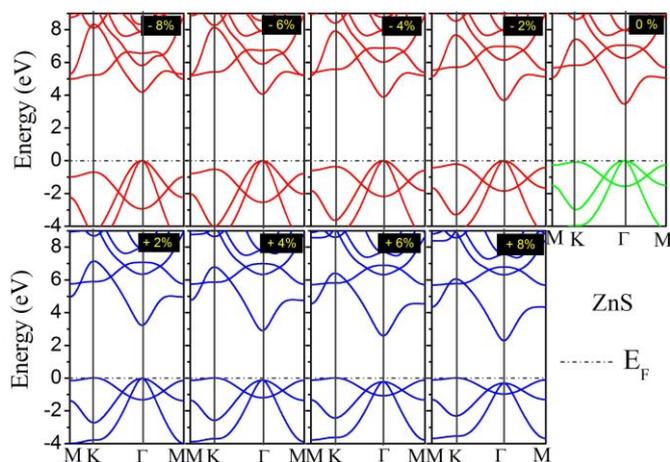


Figure 8. Calculated energy band structure of ZnS monolayer for all values of considered strain.

The band structures of the ZnSe and ZnTe monolayers under different biaxial compressive and tensile strain conditions are given in figures 9 and 10, respectively. As seen in figure 9, and figure 10, the both monolayers exhibit an indirect type band gap in free condition. According to our calculation, by applying more percent of considered tensile strain, the nature of the ZnSe and ZnTe monolayers are changed from semiconducting to metallic. Generally, exerting compressive and tensile strains has some significant effects on energy levels of these compounds. It is obvious that applying tensile strain causes to separation conduction band minimum from other levels in conduction band, so it shifts to lower energy near the Fermi level. This trend leads to energy gap reduction in tensile strain cases. The tensile strain like a perturbation factor causes to degeneracy reduction in energy levels of conduction band. In other hand, the conduction band minimum moves toward higher energy ranges by exerting compressive strain cases, the energy gap increases in these cases. Both of these effects, compressive and tensile strains, in valence band change energy situation of p_z and $px+py$ orbitals with respect to each other's.

3.3. Optical Properties

Next, we studied the optical properties on ZnO and ZnS monolayer using random phase approximation (RPA) [37]. As it is clear, HSE06 in one of the accurate method to calculate the electronic band structure of materials [38], so it is acceptable to study optical properties of our considered materials using this potential because the

optical properties of materials are related to energy levels of them.

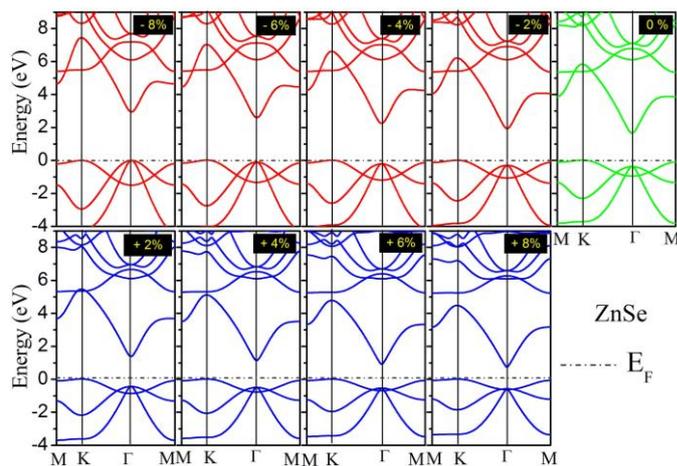


Figure 9. Calculated energy band structure of ZnSe monolayer for all values of considered strain.

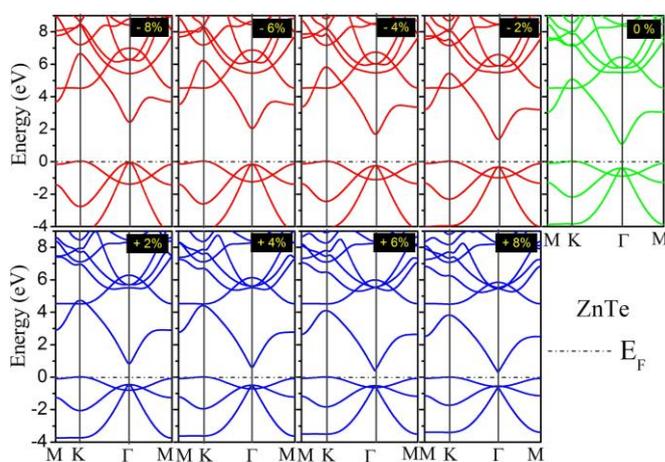


Figure 10. Calculated energy band structure of ZnTe monolayer for all values of considered strain.

The real part of dielectric function is derived from Kramers-Kronig relations [39]. Our previous works showed that exerting strain is a good strategy for engineering the optical properties of some two dimensional monolayers [40-42].

The imaginary part and optical absorption for ZnO monolayer are illustrated in the Fig. 11. Optical spectra are plotted for $\pm 8\%$, $\pm 4\%$ and free strained cases to investigate the strain effect on optical spectra. There is an anisotropy in optical spectra in both directions, $E//x$ and $E//z$ directions of incident light. This is due to the difference in bond nature Zn and O in these directions, so the energy levels have different behavior. The imaginary part of dielectric function is related to optical transition in materials, so it refers to the optical absorption spectrum. The threshold of optical absorption corresponds to optical gap in materials [39]. The obtained results expressed that the optical gap in x direction is equal to energy gap of materials in energy band structures. While, we can see a larger optical gap at z direction absorption. The thresholds of optical absorption in x direction do not have any significant

variation versus applied strain, but for z direction this spectrum experienced a red shift for tensile strain cases and a blue shift to higher energy for compressed strain systems.

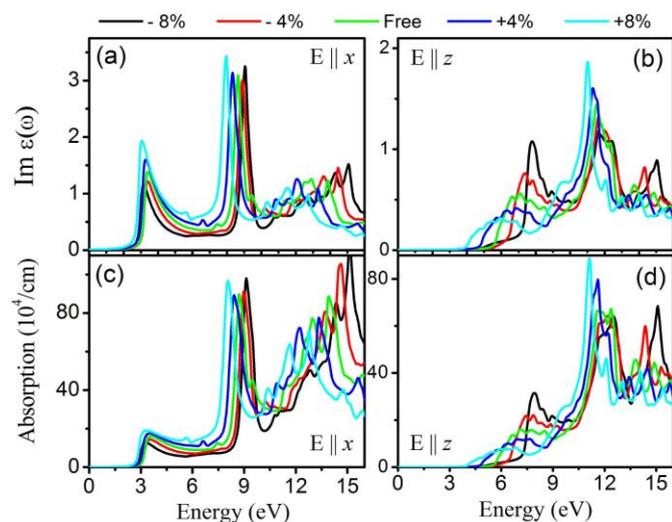


Figure 11. Imaginary part of dielectric function in (a) x and (b) z directions, Optical absorption spectrum in (a) x and (b) z directions for ZnO monolayer.

Generally, the main portion of optical absorption lies in the UV range of light. These descriptions also apply for ZnS monolayer (see Fig. 12). But, the threshold of optical absorption of this monolayer locates in the visible range. This causes a different application for ZnO monolayer. The wide gap semiconductor nanomaterials can be a good candidate to design high temperature processors. As it is clear from optical absorption spectrum in x direction (see Fig. 12c), we can tune optical gap of ZnS using exerting strain.

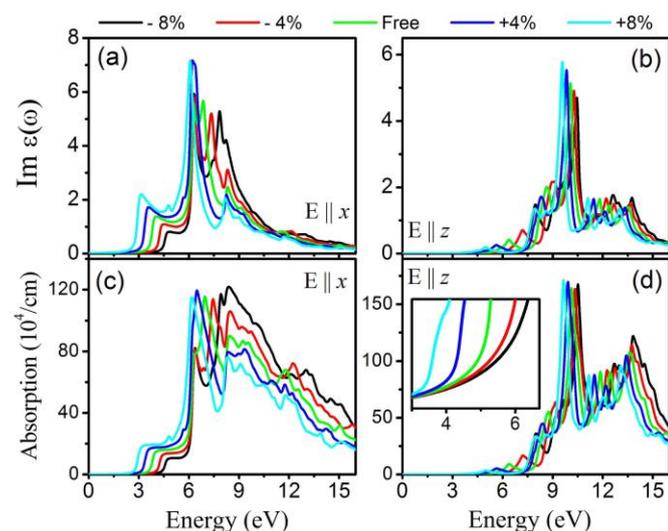


Figure 12. Imaginary part of dielectric function in (a) x and (b) z directions, Optical absorption spectrum in (a) x and (b) z directions for ZnS monolayer.

Next, the real part of dielectric function and reflectivity spectrum are calculated for both monolayers (see Fig. 13 and 14). The results exhibit that both ZnO and ZnS monolayer do not have optical absorption in the visible

light range, and the reflectivity spectra also present a reflectance about 2% in z direction of light. So, we can claim that both ZnO and ZnS monolayers are transparent nanosheets.

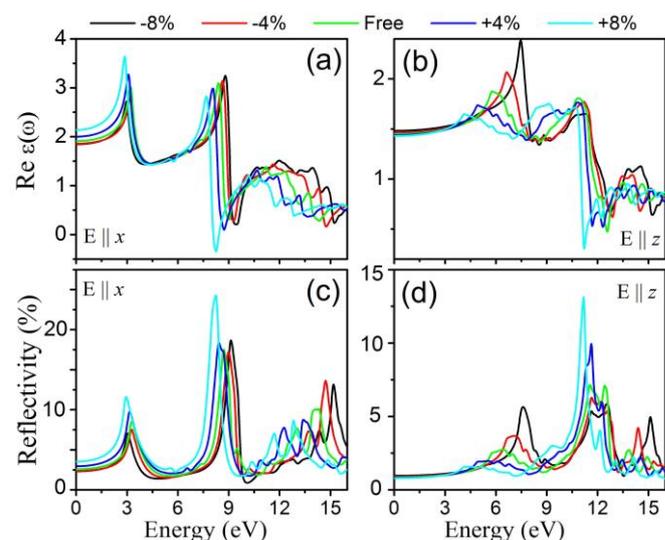


Figure 13. Real part of dielectric function in (a) x and (b) z directions, reflectivity spectrum in (a) x and (b) z directions for ZnO monolayer.

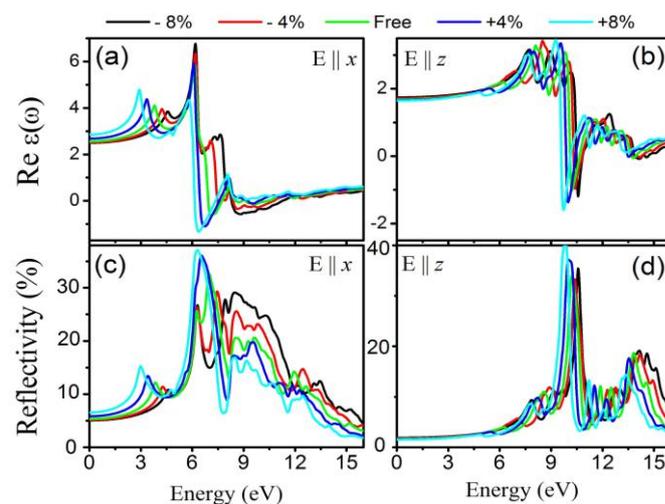


Figure 14. Real part of dielectric function in (a) x and (b) z directions, reflectivity spectrum in (a) x and (b) z directions for ZnS monolayer.

4. Conclusion

The electronic properties of ZnX ($X=O, S, Se$ and Te) graphene-like monolayers have been studied using FP LAPW+lo methods in the framework of first principles calculations. The results indicate that energy gap of these compounds can be tune using exerting biaxial strains very well. The gap variation of each compound has been interpolated versus applied strain. ZnO showed a gap reduction for both compressive and tensile strains while for the other compounds, ZnS, ZnSe and ZnTe monolayers, the energy gap increases and decreases after applying biaxial compressive and tensile strains, respectively. The energy band structure calculations illustrate that for ZnO and ZnSe the gap direction remains direct type (Γ to Γ) in compressed conditions as

well as equilibrium cases. However, the gap direction varied to $K \rightarrow \Gamma$ under tensile conditions. In ZnSe and ZnTe, the gap direction remains indirect in the whole of considered strain ranges. The electronic results exhibit that biaxial compressive and tensile strain are good strategy for controlling energy gap of considered monolayers. These results can suggest us to design new nano-base devices using two-dimensional nanostructures. Optical calculations illustrate that the optical gap and optical absorption of ZnO and ZnS nanosheets can be tune using compressive and tensile strain conditions. A red shift and blue shift for optical absorption spectra gained under tensile and compressive strain conditions, respectively. A reflectance about 2% obtained in z direction of incident light. Results of this study suggest that this type of wide gap two-dimensional monolayer can be a good candidate for high temperature processors.

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