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Buckling variation effects on optical and electronic properties of GeP$_2$S nanostructure: A first-principles calculation

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Abstract

In this study, by using the first-principles calculations based on density functional theory (DFT), the electronic aspects of GeP$_2$S monolayer under the effect of buckling variation parameter ($\mu = 0, 2, 4, 6$) are theoretically investigated by the PBE-GGA approximation method, and the obtained results have been compared with previous similar structures. We presented the imaginary part of the dielectric function and absorption spectra for in-plane and out-of-plane polarization of GeP$_2$S monolayer by PBE, HSE06, and TD-HSE06 methods. Also, optical aspects for this 2D nanostructure are presented in out-of-plane polarization under buckling variation conditions up to $\mu = 6$. It was shown that particularly for the range of visible light spectrum its optical behaviors match with its electronic ones. Consequently, the obtained results suggest GeP$_2$S as a suitable material for designing optoelectronic devices.

Key Words: first-principles calculation, buckling variation, 2D nanostructure.

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1. Introduction

The discovery of graphene has become a turning point for the beginning of extensive research on the physical properties of this structure in terms of stability, electronics, and optics with the aim of designing optoelectronic devices [1-7]. The results of studies on this 2D monolayer led to many theoretical and experimental investigations on the prediction of new nanomaterials for use in new optoelectronic devices [8-29]. Recently a new two-dimensional (2D) pristine SiP$_2$S monolayer has been predicted using the first-principles calculations [30], and then the electronic and optical aspects of SiP$_2$S under the supposed conditions have been studied by Tayran, et al. [31]. More recently, a new two-dimensional monolayer has been proposed as an indirect semiconductor with a moderate band gap called GeP$_2$S. Its structural properties such as cohesive energy and Phonon dispersions and optoelectronic properties of this monolayer under biaxial stress and strain have been investigated [32]. The buckling effect can be caused by internal forces or by external vertical compressive strains. When a structure is subjected to vertical compressive stress, buckling effects may occur [33, 34]. In this paper, by using the first-principles calculations the buckling effects on the optical and electronic aspects of the two-dimensional GeP$_2$S monolayer along out-of-plane are studied. To reach this aim, using density functional theory (DFT), we first obtain the electronic and optical properties of the GeP$_2$S monolayer with a buckling variation parameter equal to zero. Then, as an alternative method, we present some optical aspects such as the imaginary part of the dielectric function and the absorption spectra with the time-dependent density functional theory (TDDFT) based on the hybrid exchange-correlation function with the TD-HSE06 method [35]. Then its properties under different buckling situations, which are induced by compressive vertical strains, along out-of-plane the monolayer are studied.

This paper is prepared as follows:

In the next section, Calculation and simulation methods are presented. The structural and stability of the GeP$_2$S 2D monolayer are discussed in Section 3. The electronic and optical
properties of this monolayer under buckling effects are given in Sections 4 and 5, respectively. Finally, in the last section, the paper is summarized.

2. Calculation methods

The computational method in this paper is based on the first-principles calculation on the basis of density functional theory. The optimized ground state and dynamic stability of the GeP₂S monolayer have been calculated using the QUANTUM ESPRESSO package [36]. In these tasks, the cutoff energy is supposed to be 60 Ry for expanding the valence electrons wave functions. The electronic and optical properties of this monolayer under buckling variation conditions up to \( \mu = 6 \), were obtained by applying density functional theory implemented in Wien2k simulation code [37]. The complete potential linear augmented plane waves plus local orbital (FPLAPW+LO) method was employed for the extension of the Kohn-sham wave function. The exchange-correlation term is produced by utilizing the generalized gradient approximation represented by Perdew–Burke–Ernzerhof (GGA-PBE) [38]. Also to get more accurate band gaps, the electronic band structures calculations have been done on the basis of hybrid functional theory by Heyd-Scuseria-Ernzerhof (HSE06) approximation method [39]. For electronic and optical measures, the Monkhorst-Pack approximation was initially applied to the Brillouin zone (BZ) with \( k \)-point meshes \( 12 \times 12 \times 1 \) and \( 25 \times 25 \times 1 \) [40]. Computational input parameters for computing have been considered to calculate the electronic properties multiplied by the product of the smallest atomic sphere radius times the largest K-vector of the plane wave expansion of the wave function \( R_{MTK_{\text{max}}} = 7 \), the magnitude of the largest vector of the plane-wave cutoff \( G_{\text{max}} = 14 \text{ Ry}^{1/2} \), and the angular function’s value \( l_{\text{max}} = 10 \). Computational input parameters have been considered to calculate the electronic properties multiplied by the smallest radius of the atomic sphere at the largest emission vector \( K \), the function \( R_{MTK_{\text{max}}} = 7 \), the magnitude of the largest waveform, and the angular function. The energy to separate the core from the valence electrons is chosen as \(-8\text{Ry}\), the calculations are performed for the un-polarized spin configurations. The Kramers-Kronig relations and the random phase approximation (RPA)
method are also applied to gain the complex dielectric function components of 2D GeP$_2$S nanostructure, obtained from interband transitions [41]. We utilize the time-dependent density-functional theory (TDDFT) calculations using the Casida equation [35]. The numbers of valence and conduction bands employed for expanding two-particle wave functions in TDDFT are $(6v, 6c)$. To obtain converged spectra, the k-meshes are determined to be $avg - (12, 8)$. We are using the TD-HSE06 method to study effectively predict excitonic transitions effects in optical absorbance spectra of GeP$_2$S. The 8 occupied and 16 unoccupied states with $12 \times 12 \times 1$ and $6 \times 6 \times 1$ $k$-point meshes have been applied in the TD-HSE06 calculations on the GeP$_2$S monolayer.

3. Structural properties and the stability

The optimized GeP$_2$S monolayer, as a 2D crystalline nanostructure with a rectangular atomic configuration, is shown in Figure 1. The side-view of the GeP$_2$S monolayer is also shown in figure 1 (a), where $\delta$ is the buckling distance parameter, which denotes the normal vertical distance between the upper and lower layer of germanium and phosphorus atoms which is equal to the total thickness of the 2D GeP$_2$S monolayer. The top views of GeP$_2$S supercell and unit cell consideration are shown in figure 1 (b), (c) [32].

Figure1: (a),(b) side-view and top view of supercell (c) unit cell, and (d) Energy vs Volume unit cell of GeP$_2$S.
The lattice constants of the GeP$_2$S are optimized by using the thermodynamical equation state of Birch-Murnaghan [42]:

$$E(V) = E_0 + \frac{9B_0 V_0}{16} \left\{ \left( \frac{V_0}{V} \right)^{2/3} - 1 \right\}^3 B_0' + \frac{9B_0 V_0}{16} \left\{ \left( \frac{V_0}{V} \right)^{2/3} - 1 \right\}^2 \left[ 6 - 4 \left( \frac{V_0}{V} \right)^{2/3} \right] \right\}$$ (1)

According to Equation (1), the energy for the optimized volume is obtained with the lattice parameters (a, b) where $V_0$ is the initial volume, $B_0$ represents the bulk modulus without pressure and $B_0'$ derives the bulk modulus of the pressure. Figure 1 (d), is shown the energy vs volume curve for the optimized GeP$_2$S unit cell. According to this figure, the minimum point of this curve demonstrates the optimized volume in minimal energy of the unit cell. Following the obtained equilibrium volume, the optimized lattice parameters are proposed as $a = 4.756\,\text{Å}$, and $b = 3.35\,\text{Å}$ and $\delta = 2.18\,\text{Å}$. The Results of structural properties investigation in this study designate that optimized 2D GeP$_2$S nanostructure is an indirect bandgap semiconductor with 0.681 eV value for PBE method and 1.367eV calculated by HSE06 approximation method.

Table 1 display the optimized structural data of GeP$_2$S monolayer such as lattice parameter, buckling distance, and optimized bandgap energy using PBE-GGA approximation method [32] and compared with structural data of two samples of 2D nanostructures called Penta-graphene[34] and SiP$_2$S [30].

| Structure           | Optimized lattice (Å) | Buckling (Å) | $E_g$ (eV) | Type       |
|---------------------|-----------------------|--------------|-----------|------------|
| Penta-graphene      | $a = b = 3.649$       | $\delta = 1.178$ | 2.23      | Indirect   |
| SiP$_2$S            | $a = 4.79\,\text{, } b = 3.296$ | $\delta = 2.12$ | 0.52      | Indirect   |
| GeP$_2$S (This work)| $a = 4.756\,\text{, } b = 3.35$ | $\delta = 2.18$ | 0.68      | Indirect   |

Table 1: optimized structural data, lattice parameter, buckling distance, and bandgap energy of GeP$_2$S and similar monolayers by PBE-GGA method [30, 31, and 34].
Moreover, electronic and optical aspects of GeP$_2$S monolayer under various buckling vertical compressive conditions were studied in this case. The vertical compressive strain values for GeP$_2$S were executed to the buckling distance parameter ($\delta$) as the values of buckling parameter variations for this investigation cases are given by: the buckling variation parameter is defined by $\mu$ which refers to the ground state buckling distance ($\delta$) by

$$\delta_\mu = \left(1 - \frac{\mu}{100}\right) \delta_{eq} \quad (2)$$

Where $\delta_{eq}$ the equilibrium buckling distance is the unstrained structure buckling distance, $\mu$ is the value of vertical compressive strain which in this study is considered as $\mu = 0, 2, 4, 6$

For more study, before studying the electronic and optical properties of GeP$_2$S unit cell under buckling compressive strain conditions, the total energy and bandgap was calculated under buckling parameter variations up to $\mu = 6$, and have been compared with SiP$_2$S monolayer values [31]. According to Figure 2 (a), The calculation bandgap variations under the effect of buckling compressive strain by PBE-GGA and HSE06 approximation methods have been illustrated by blue and red curves, which show that the bandgap decreases by imposing buckling strain up to $\mu = 6$. The stability of the GeP$_2$S monolayer reduces slightly, according to Figure 2 (b). In addition, to better understand the concepts and validation, the results of this study have been compared with the SiP$_2$S monolayer under the same conditions. This comparison shows that the behavioral variations of GeP$_2$S in the assumed conditions have an acceptable agreement with the structural behavior and energy of the SiP$_2$S monolayer, as shown in Figure 2.
4. Electronic properties

In this section, the energy band structure and total density of states for the optimized GeP$_2$S monolayer have been investigated to determine the concentration of electrons and holes as a function of energy and the probability that each of these levels is occupied and compared with optimized SiP$_2$S monolayer by hybrid functional theory (HSE06), and PBE-GGA approximation methods. Figure 3 (a) illustrates the band structure and total density of states of GeP$_2$S and the atoms forming the two-dimensional nanostructured unit cell. According to Figure 3(a), the optimized GeP$_2$S nanostructure is presented as an indirect bandgap semiconductor with the value of 1.367 eV by HSE06 and 0.681 eV by PBE-GGA approximation method, which is between valence band maximum (VBM) and conduction band minimum (CBM) on the Γ-Y points. The charge concentration analysis of the projected total DOS indicates the high electron density of the GeP$_2$S unit cell in the valence and conduction bands. The total DOS for each atom shows that the electron density of phosphorus atoms around VBM is greater than that of germanium and sulfur atoms. Also, the comparison of the energy band structure results obtained for this monolayer [32] with the previous outcomes of similar structures such as SiP$_2$S [31] shown in Figure 3(b) indicates the reliability of the calculations performed in this study.
In the sequel, as a significant effect in designing the electronic devices by using 2D materials, the buckling effects on the electronic aspects of GeP$_2$S monolayer have been studied. Plots of the energy band structure and total density of states of GeP$_2$S monolayer under the influence of buckling vertical compressing up to $\mu = 6$ are indicated in Figure 4. As shown in this figure under buckling compressive strain conditions, the indirect bandgap of this semiconductor was calculated by PBE-GGA approximation method with 0.681 eV energy value, for $\mu = 2$ & 4, decreases to 0.61 and 0.56 eV values respectively and remains as indirect bandgap between VBM and CBM in $\Gamma$-Y points. In $\mu = 6$, the bandgap reduces up to 0.496 eV, while the indirect bandgap shifts to between X- $\Gamma$ to Y-F path.
5. Optical properties

In this section, under the conditions of buckling variation ($\mu = 0, 2, 4, 6$), optical properties of GeP$_2$S such as optical joint density of states (joint DOS), real and imaginary parts of the complex dielectric function, absorption, reflectivity, and energy loss are investigated.

The first optical aspect we consider in this section is the optical joint density of states, which represents the density of the states $q(\mathbf{v})$ of a photon of energy, $\hbar \nu$ under energy conditions that interact with momentum conservation in a direct-gap semiconductor. This quantity is a combination of the density of the states in both the valence and conduction bands. The Optical joint density of states is expressed by the following equation [43]:

$$q(\mathbf{v}) = \frac{(2m_r)^{2/3}}{\pi \hbar} (\hbar \nu - E_g)^{1/2}, \quad \hbar \nu \geq E_g$$  \hspace{1cm} (4)

At the first step, to study optical band- to- band (interband) transitions from the occupied states to the unoccupied states, the optical joint DOS plots of the optimized GeP$_2$S monolayer in X, Y, and Z polarization directions using the PBE-GGA approximation method, has been plotted in

![Figure 4: The energy band structure plots of the GeP$_2$S under the effect of buckling strain conditions.](image)
Figure 5. The optical bandgap due to the first optical transition in each direction is determined by the threshold of the joint DOS graph.

Fig. 5 (a) shows the joint density of states for optical interband transitions in the armchair, zigzag and out-of-plane directions. The main transition peak in the X and Y polarization directions appears at 1.09 eV and 1.23 eV, respectively, which correspond to the optical bandgap. While the prominent transition peaks in the Z polarization direction occur around 5 -7 eV. The four major transition peaks for each polarization direction are compared in Figure 5 (b).

Complex dielectric function is a physical concept for deriving the significant optical aspects such as absorption, refractive index, and reflectivity as a function of frequency which contains two components, real and imaginary parts as following equation:

$$\varepsilon_{\text{complex}} = \varepsilon_1 + i \varepsilon_2$$

(5)

Where $\varepsilon_1$, epresents the real part of the dielectric function obtained by Kramers-Kronig with the following relation:

$$\varepsilon_1^{\alpha\beta}(\omega) = \delta_{\alpha\beta} + \frac{2}{\pi} \text{Pr.} \int_0^{\infty} \frac{\varepsilon^{\alpha\beta}(\omega')}{\omega'^2 - \omega^2} \omega' d\omega'$$

(6)

Where Pr. applies the Cauchy principal value to the integral of the equation.
Subsequently, \( \varepsilon_2 \) represents the imaginary part of the complex dielectric function which is considered an effective factor in the optical interband band transmissions between occupied \((ik)\), and unoccupied \((fk)\) electron states, and follows the equation [45]:

\[
\varepsilon_2^{\alpha\beta}(\omega) = \frac{4\pi e^2}{m^* \omega^2} \sum_{i,j} \int \frac{d^3 k}{(2\pi)^3} |\langle ik | P_\alpha | fk \rangle|^2 f_i^{k}(1 - f_j^{k}) \delta(E_f^{k} - E_i^{k} - \hbar \omega)
\]

In the calculation of the optical properties of a semiconductor, several types of energy transitions occur, such as band-to-band (inter-band) transitions, free-carrier (intraband) transitions, phonon transitions, and excitonic transitions. In the PBE and HSE06 approximation method, the effect of excitation on the transition energies is ignored, while in the TD-HSE06 method this effect is taken into account in the transition energies calculations. To achieve more accurately the energy transitions calculations in the optical spectra, in addition to the PBE and HSE06 approximation methods, we use time-dependent density-functional theory (TDDFT) based on hybrid exchange-correlation functional is produced by utilizing the TD-HSE06 approximation method which involves the essential ingredients of electron-hole interactions in its formalism in contrast to its local/semi-local functional counterparts and formulated as a generalized eigenvalue equation called the Casida equation [35].

Figure 6: The imaginary part of the dielectric function of GeP₂S calculated by PBE, HSE06 and TD-HSE06 for in-plane X (a), Y (b) and out-of-plane Z (c) direction polarization.
Figure 6, demonstrates the imaginary spectra of the dielectric function in-plane X and Y directions and out-of-plane Z polarization, by independent particle PBE and HSE06 approximation, and TD-HSE06 method as a subsequent step to HSE06 calculations \[44\]. We note that the absorption of a photon can result in the formation of an electron and a hole at some distance from each other but which are nevertheless bound together by their mutual Coulomb interaction. This entity, which is much like a hydrogen atom but with a hole rather than a proton, is called an exciton. A photon may be emitted as a result of the electron and hole recombining, thereby annihilating the exciton \[43\]. TD-HSE06 method is moderate computational cost and effectively accounts for excitons \[45\]. According to Figure 6, it can be seen that for in-plane armchair and zigzag polarization directions in the optical spectrum from 1 to 5 eV, by applying the excitation transitions effect, we are faced with a significant decrease in the imaginary spectra peaks, especially in contrast to PBE method and optical band gap is shifted to higher energy, while in Z-direction under the effect of excitation with TD-HSE06 method in the range of optical band gap (1.3 eV), and the increasing peak is observed compared to time-independent approximation methods, especially compared to the PBE method.

The optical absorption spectra as a major part of imaginary spectra of the dielectric function are also calculated by PBE, HSE06, and TD-HSE06 approximation methods for in-plane X, Y, and out-of-plane Z-direction polarization GeP$_2$S monolayer and have been demonstrated in Figure 7.

Figure 7: In-plane optical absorbance computed with the TD-HSE06 method, HSE06 functional, and PBE functional in armchair direction (a), zigzag path (b), and out-of-plane optical absorbance Z direction (c).
Since we assume GeP$_2$S as a 2D nanostructure positioned at X-Y plane, for buckling variation effects, we only investigated its optical responses in for the incident lights along out-of-plane Z direction (normal to its surface).

For investigation of the optical interband transition from the occupied states to the unoccupied states, the joint DOS plots of GeP$_2$S monolayer Z polarization direction for buckling parameter variations up to $\mu = 6$ in Z direction polarization are computed and presented in Figure 8.

![Joint density of states (DOS) of GeP$_2$S in the Z direction for buckling parameter variations up to $\mu$=6.](image)

According to the figure, except for the energy range of 5.6 eV, which can be observed a sharp peak for $\mu = 6$, elsewhere in the energy interval (0- 10 eV), especially in the frequency range of the visible light spectrum (1.5 to 4 eV) under the influence of fluctuating the buckling parameter up to $\mu = 6$. The optical transition behaviors in the joint DOS diagram are regular and do not change abruptly, a representative that this monolayer is appropriate for optical applications under the conditions considered in this study.
According to Figure 9, the real and imaginary plots of the complex dielectric function of GeP$_2$S monolayer in Z direction polarization, under buckling parameter variations up to $\mu = 6$, are plotted.

![Figure 9: (a) real and (b) imaginary part of the dielectric function of GeP$_2$S under buckling variation.](image_url)

According to Figure 9 (a), the real part of the dielectric function under the effect of buckling parameter variations up to $\mu = 6$ is slightly shifted to upper energies. The imaginary section of the complex dielectric function for Z-direction under the considered conditions is plotted in Figure 9 (b). The main peak in these graphs is related to the optical absorption between the valence and conduction band state in the Z-polarization directions. It should be noted that imaginary plots under the conditions of buckling variations in the optical energy range, especially in the visible light spectrum (1.5 to 4 eV), similar to the real part diagrams, have smooth shifts and normal behavior.
The absorption and reflectivity have two significant properties for studying the optical aspects, which can be concluded in terms of the real and imaginary parts of the complex dielectric function. The absorption and reflectivity under buckling vertical compressive strain conditions with Z-polarization direction have been plotted in Figure 10. As shown in Figures 10(a) and (b), by applying buckling parameter variations up to $\mu = 6$, the intensity of absorption and reflectivity spectrums faintly is increased in comparison with the free-state. The absorption peaks for $\mu = 2, 4 \& 6$, are shifted to the higher intensities around 6 to 7 eV. Under-considered conditions of this study, it can be observed a relative and regular shifting on the absorption and reflectivity spectrums, particularly in the interval of visible light energy. It can be said that the GeP$_2$S monolayer has acceptable light stability in these conditions, and this material can be considered suitable for use in optical devices, especially in optoelectronic sensors.

![Figure 10: (a) Absorption & (b) Reflectivity spectrum of GeP$_2$S monolayer; for $\mu = 0, 2, 4 \& 6$.](image-url)
As the last point, the energy loss (ELOSS) was investigated. Figure 11, shows the ELOSS spectrum of the GeP₂S monolayer in the 0-20 eV energy under vertical buckling compressive conditions. The maximum peak of the ELOSS spectrum specifies the plasma frequency. According to the figure, the plasma frequency of the GeP₂S is detected at 12.4 eV. And this value by applying the buckling compressive effects is slightly shifted to higher intensity, and finally, for $\mu = 6$, the plasma frequency occurs about 13 eV. As expected, similar to other optical aspects, in the ELOSS under the conditions considered in this study, imperceptible changes with very low intensity are observed in the visible light spectrum.

![Figure 11: ELOSS spectrum of GeP₂S monolayer; for $\mu=0, 2, 4 & 6$.](image-url)
6. Conclusions

In a nutshell, the electronic and optical properties of the GeP$_2$S as a two-dimensional nanostructure based on first-principles calculation in the framework of density functional theory (DFT), were investigated under the buckling vertical strain. Analyzing the electronic properties such as band structure under four selected buckling variation parameters ($\mu = 0, 2, 4, 6$) indicates that the energy band gap of GeP$_2$S as an indirect bandgap semiconductor declines moderately from 0.681 eV to 0.496 eV when the buckling variation goes up from $\mu= 0$ to $\mu= 6$. The imaginary part of the dielectric function and optical absorption spectra have been studied by PBE, HSE06, and TD-HSE06 approximation methods. The study of GeP$_2$S monolayer optical aspects under buckling variation, especially in the visible light spectrum, indicates minor and regular fluctuations, which can be suggested this monolayer as a suitable option for designing electro-optical devices, especially optical sensors.

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Code availability: Not applicable.

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