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Electronic and optical properties of beryllium sulfide monolayer: Under stress and strain conditions

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ABSTRACT

Electronic and optical properties of two-dimensional graphene-like structure of beryllium sulfide (BeS) have been studied in the framework of the density functional theory. Different values of stress and strain are exerted for tuning electronic and optical parameters. The electronic results show that both biaxial stress and strain effects cause band gap reduction with different rates. Also, we have red and blue shifts in the optical absorption spectrum peaks by applying strain and stress, respectively. Our results express that BeS monolayer can be the promising candidate for the future nano-devices.

1. Introduction

Vigorous research on graphene and its applications [1,2] has created a fertile ground for the investigation of a broad range of alternative two-dimensional nanomaterials. In the last decade, many groups of two-dimensional semiconductor nanomaterials were studied and applied in the different fields of industry. Some of more famous materials are BN [3,5,4], SiC [6,7], transition metal dichalcogenides [8,9], black phosphorus (BP) [10,11] and zinc oxide [12,13]. Among these categories of nanomaterials, two-dimensional II–VI semiconductors have been studied by different groups. Their results presented that these materials in graphene-like structure have a good structural stability [14]. Also, the electronic and optical properties of family of these two-dimensional materials have been studied by computational and experimental approaches [15–17]. Yu and Guo studied two-dimensional beryllium sulfide (BeS) by first principles calculations [18]. They found that this monolayer has a good thermodynamical stability up to 1000 K and is a wide gap semiconductor about of 4.26 eV. Also, they found that armchair edge BeS nanoribbon has semiconducting properties while the zigzag edge is a ferromagnetic metal. Recently, An and colleagues investigated electronic transport properties of graphene-like beryllium sulfide nanoribbons [19]. They obtained that the electrons flow mainly through the two edges of zigzag BeS nanoribbon and they presented that BeS nanoribbon can be the promising candidate for the future nano-devices.

On the other hand, exerting stress and strain is one of the effective way to control electronic and optical properties of two-dimensional materials. Liu and colleagues studied applying biaxial stress and strain on electronic properties of AlN nanosheet [20]. They claimed that in some values of shear strain along the zigzag direction induces an indirect-to-direct transition in band gap. Different kind of behavior was reported for ZnO graphene-like structure by Kaewmaraya et al. [21]. Their results illustrated that the band gap of the sheet varies almost linearly with uniaxial strain while it shows a parabola-like behavior under homogeneous biaxial strain. Similar studies are performed for different two-dimensional materials by first principles calculations [13,22,23].

Hence, we decided to study electronic and optical properties of BeS monolayer by first principles calculations to find more potential applications for this compound. These properties are studied under different biaxial stress and strain conditions.

2. Computational details

Electronic and optical properties of beryllium sulfide monolayer have been investigated using first principles study calculations in the framework of the density functional theory as implemented WIEN2k code [24]. Full potential augmented plane waves plus local orbital (FPAPW + *lo*) has been used to expand basis set functions. The exchange-correlation potential has been treated using generalized gradient approximation presented by Perdew–Burke–

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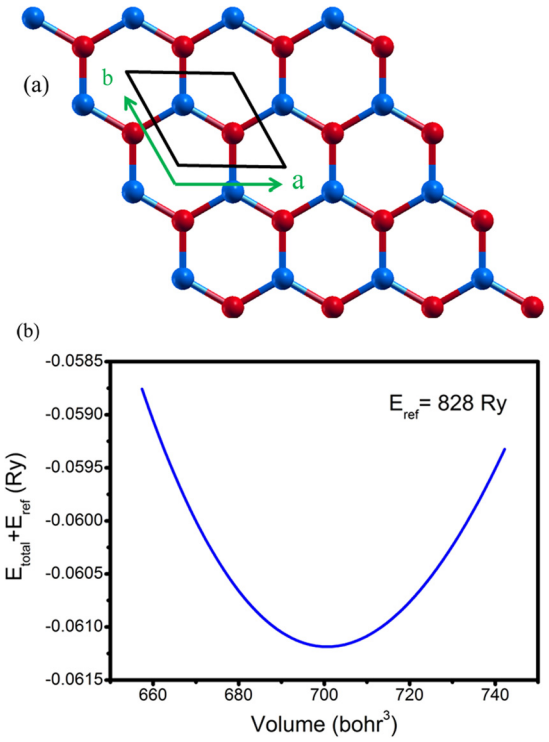

Fig. 1. (a) The unit call of honeycomb structure of BeS monolayer and its lattice vector, (b) The E–V curve of BeS monolayer.

Ernzerhof (GGA-PBE) [25]. The value of optimized input parameters in our calculations are $R_{MT}K_{max} = 8$ and $l_{max} = 10$. The Fourier expansion of electron charge density is expanded by $G_{max} = 14$ Ry$^{1/2}$. The convergence criteria in optimization and electronic calculations were set to $|E_{i+1} - E_i| \leq 10^{-4}$ Ry on energy of system and $|\rho_{i+1} - \rho_i| \leq 10^{-5}$ on electron charge, respectively. Vacuum spacing is arranged so that the minimum distance between two monolayer in adjacent unit cells is about 15 Å, provided that atoms have negligible interaction at that far distance. Based on Monkhorst–Pack scheme [26], $15 \times 15 \times 3$ and $35 \times 35 \times 7$ k-meshes have been considered in the whole of first Brillouin zone to calculate electronic and optical properties, respectively. The optical data of this paper has been performed by the random phase approximation (RPA) method [27] to gain imaginary part of dielectric function and Kramers–Kronig relations for the real part.

3. Results and discussion

3.1. Structural properties

In order to find structural stability of graphene-like structure of beryllium sulfide monolayer (see Fig. 1a), the total energy of compound versus unit cell volume has been calculated using thermodynamical Brich–Murnaghan equation of state [28]:

$$E(V) = E_0 + \frac{9B_0V_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^3 B_0'\right\} + \frac{9B_0V_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^2\left[6 - 4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\} \quad (1)$$

where V_0 is the initial considered volume, V is the deformed volume, B_0 is the bulk modulus, and B_0' is the derivative of the bulk modulus with respect to pressure. This formula presented the variations of total energy of system versus the unit cell volume. We optimized the lattice constant of BeS monolayer (see Fig. 1b). The obtained equilibrium lattice constant is $a = b = 3.45$ Å that is in good agreement with previous calculations [18]. After optimizing lattice constants, the force relaxation calculation has been performed to achieve the equilibrium atomic positions. We have found the atomic positions of beryllium and sulfur atoms are completely similar to other graphene-like structures, Be$(1/3, 2/3, 0)$ and S$(2/3, 1/3, 0)$. Also, the relaxation process present that this structure is completely flat and there is not any planar buckling.

After these steps, we exerted different values of stress and strain to investigate the variation of electronic and optical properties of BeS monolayer under different structural conditions. Considered values are:

$$a_{\pm\delta} = \left(1 \pm \frac{\delta}{100}\right) a_{eq} \ , \quad (2)$$

where $\delta = 2$, 4, 6 and 8, a_{eq} is the equilibrium lattice constant (free-strain lattice constant) and the positive and negative signs refer to strained and stressed cases, respectively.

3.2. Electronic properties

Electronic property is an important part for every compound investigations. In fact, it helps us improve our rough understanding about compounds' electrical behavior into an acceptable level. "Beryllium" as one of the elements of group II of periodic table can contribute in ionic-covalent bond especially with "sulfur" element. In order to identify the characterization of this compound, we have calculated the fractional ionic character (FIC). This factor can be calculated by formula (1) as it was represented by Xu and Ching for calculation the contribution of ionic and covalent bonds in binary compounds [29].

$$FIC = \left|\frac{Q_{Be} - Q_S}{Q_{Be} + Q_S}\right| \times 100 \ , \quad (3)$$

where Q_{Be} is affective charge of beryllium that has participated in Be–S bond, and Q_S is sulfur's simultaneously. Obviously, this factor can be represented between 100% and 0%, which denote to ionic and covalent natures, respectively. The fractional ionic character for the Be–S bond is 65% and shows that it keeps covalent nature a bit, yet the ionic nature is more than covalent nature here.

Investigating density of states of electrons compared with band structure graph tells us electronic properties of this structure in general. These two graphs are illustrated in Fig. 2. Recognizing its semiconducting property as a consequence of band gap existence is the first point to mention. Band gap value of this nanosheet is about 4.55 eV. On the other hand, its wide band gap is indirect type in $K \rightarrow M$ direction and tells us how electron transition may occur in electrical conductivity process as well. Clearly, it can be considered as a good agreement with previous data that approves our calculation in general [18].

Moreover, investigation of the partial density of states in Fig. 3 brings about a good view about the main orbitals around the Fermi level. These orbitals simultaneously play a main role in electrical conductivity of compounds. Clearly, s and p orbitals which are situated in almost the similar region of energy, create density of states around the Fermi level. As it is clear from Fig. 3c and 3d, the edge of conduction band minimum (CBM) and of valence band maximum (VBM) are created by p_z known as π and π^* orbitals of sulfur and beryllium, so it demonstrates that electrical conductivity mostly move through these orbitals after supplying voltage. While the $p_x + p_y$ stays in plane to create sp^2 hybridized orbitals with s orbital.

One of the most important parts of the investigation of every compound is to study the effect of external forces on them such as substrate effect, supplying substrate effect and so on. We