Prediction of Electronic and Optical Properties of Boron Selenide BSe (2H) monolayer based on First-Principles

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Abstract. In this study, we examined some properties of 2D monolayer of Boron selenide BSe (2H) such as structural, electronic and optical properties. The BSe (2H) monolayer has an indirect bandgap of 2.62eV from Γ to M points. We explored from density of states (DOS), in valance band close to fermi level 4p state of selenium (Se) atom is hybridized with 2p state of B atom, but close to lower part of conduction band 2p state of boron (B) atom is ascendant over the 4p state of selenium atom. We have also calculated optical parameter like imaginary and real component of dielectric function, refractive index, absorption coefficient from random phase approximation method(RPA).

Introduction

Due to their interesting electrical, optical, thermal and mechanical properties 2D materials have gained much attention in recent years; which allows for more versatile future applications in nano-electronic devices [1-4]. The search of new 2D materials is still a top main target of material researcher, since of their surface area is high and ability to tune the properties [5,6]. Recently baron-based chalcogenides, in the form of 2D monolayer, analogues to indium selenide [7] are attracting a lot of interest because their special properties greater stretchability, tensile strength [8], and high carrier mobility [9]. BS, BSe and BTe are three popular boron monochalcogenides. They are mainly found in two type of atomic structures 1T and 2H. In 1T structure ABBC type of atomic layers sequence found, and in 2H structure ABBA type of atomic layer sequence is obtained.
In this study, we examined structural, electronic, and optical properties of boron selenide BSe (2H) monolayer by utilizing first principle calculations.

Methodology

The density functional theory was used in all of the simulations and have been executed in the Vienna Ab-into Simulation Package (VASP) code [10]. We choose pseudopotential, projector augmented wave (PAW) and generalized gradient approximation GGA-PBE method suggested by Perdew et.al [11] was used to deal with exchange correlation energy. For plane wave basis set, we select cut off 500 eV. The force and energy convergence level were set at 0.005 eV/Å and 10^{-5} eV. For optimization using the Mon-khorst-pack scheme [12] the k-points for Brillouin Zone sample size is given as 19x19x1. We have given 15Å vacuum in vertical direction to avoid the possibility of interaction between two layers. For investigating optical properties, we have used random phase approximation (RPA) method [13]. In order to display atomic structure, the VESTA [14] code was used.

Results and Discussions

Structure properties

Figure1 depicts the completely optimised structure of boron selenide BSe (2H) monolayer. It is made of two buckled BSe layers of that are joined in such a way that two B atoms are sandwiched between Se atoms. The calculated bond length B-Se is 2.10Å and lattice constant, a = 3.25Å. The bond length after optimization, between top B atom and bottom B atom (fig. 1(b)) is 1.71Å. Similarly, the distance between upper and lower Se atom (fig.1 (b)) is 3.60Å. The calculated bond angles are ∠BSeB = 101.34° ∠SeBSe = 101.34° ∠SeBB = 116.72°. The buckling parameter is 0.95Å, this is in accordance with previous work [8].
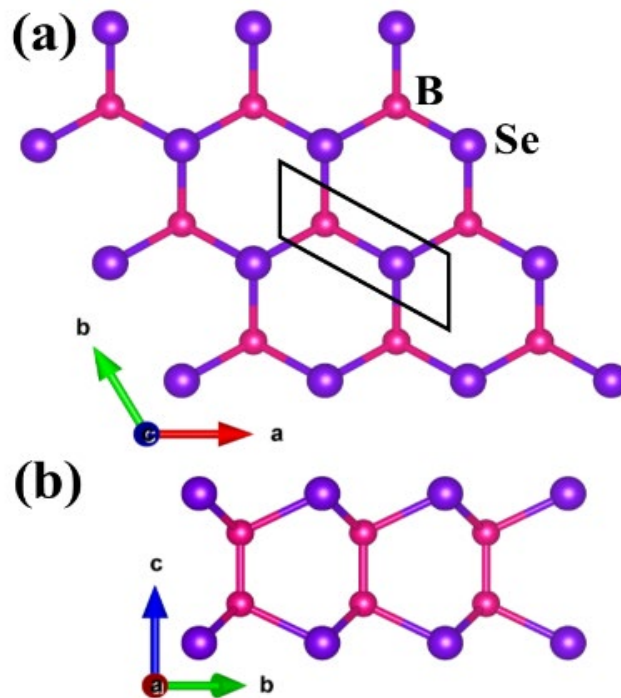

Figure 1. Optimised structure of 2D boron selenide BSe (2H), (a)
top view (b) side view.

Electronic properties

For investigation of electronic properties, we have calculated band structure and density of states (DOS) for boron selenide BS (2H) monolayer. From fig. 2(a) we obtained the indirect band gap of 2.62 eV along Γ to M direction. As shown in fig. 2(b) density of states. In valance band near fermi level, p state of Se atom ascendant over all states. But close to the lower part of conduction band p state of B atom ascendant over the all states. This demonstrates that an electron transition will occur between the p state of Se and the p state of B atom mainly. Although away from the conduction band p state of B atom is hybridized with p state of Se atom. Meanwhile in valance band away from fermi energy p state of Se atom is not hybridized with p state of B atom. Besides the s states of B atom and Se atom have very less contribution in density of sates (DOS) of BSe (2H) monolayer.
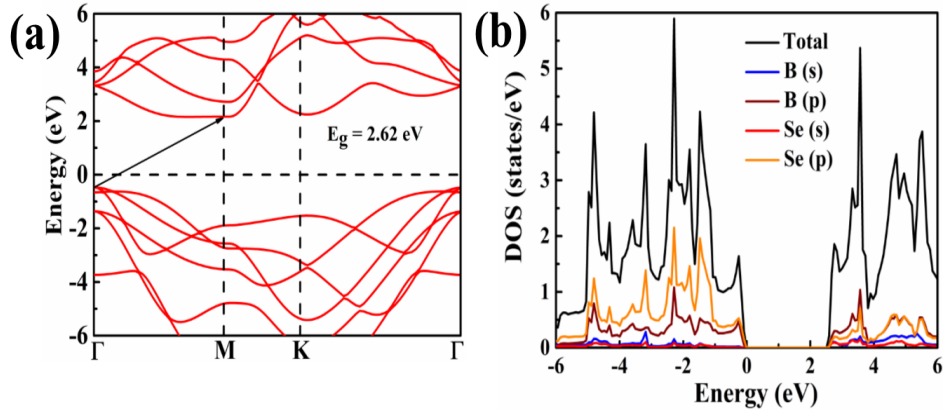
*Figure 2. (a) and (b) represents band structure and density of states (DOS)
of boron selenide BSe (2H) monolayer*

Optical properties

We used random phase approximation (RPA) method to determine imaginary and real parts of complex dielectric function for optical properties calculation. The complex dielectric function $\varepsilon(\omega)$, is defined as $\varepsilon(\omega) = \varepsilon_r(\omega) + i\varepsilon_i(\omega)$ where $\varepsilon_r(\omega)$ is real part and $\varepsilon_i(\omega)$ imaginary part of dielectric function of BSe (2H) monolayer. The optical properties have been determined in both directions in plane of polarisation (E||X) and perpendicular to plane of polarisation (E||Z). Fig. 3 represents the optical properties of BSe (2H) monolayer

Fig. 3(a) illustrate $\varepsilon_i(\omega)$ frequency dependent imaginary part of dielectric function vs photon energy. When a material is transparent for particular photon energy, the imaginary dielectric function $\varepsilon_i(\omega)$, became zero, but when absorption begins, the imaginary dielectric function turns non-zero. For E||X, imaginary dielectric function nearly zero till 1.70 eV, after 1.70eV absorption started reached maximum at 5.83 eV and become zero again after 35.0 eV. That is suggested that absorption occurs between 1.70eV and 35 eV, which can also be seen in Fig. 3(d). For E||Z, $\varepsilon_i(\omega)$, remains zero till 4.2 eV and reaches maximum at 18.52 eV, and after 35.0 eV tuns to zero. That implying material is transparent for less than 4.2 eV and more than 35 eV.

According to fig. 3(b) which shows the graph between real part of dielectric constant $\varepsilon_r(\omega)$ and photon energy. $\varepsilon_r(\omega)$ describes how much a material becomes polarised when an electric field is applied due to the formation of electric dipoles. At zero energy the value of $\varepsilon_r(\omega)$ is considered as static dielectric function. From fig. 3(b), the determined static dielectric function is 4.11 for E||X and 1.58 for E||Z, which is asserting the material have high polarizability in X direction [15].

Figure 3(c) represents how does material's refractive index connect with photon energy. Static refractive index is 2.02 for E||X, and 1.04 for E||Z. It is obvious from fig. 3(c) refractive index begins 0eV reaches highest value 2.71 at 4.76 eV (E||X), 1.44 at 17.5 eV (E||Z) after this graph decreases gradually and reached at minimum value 0.50 at 13.03 eV(E||X) and 0.75 at 23.42 eV (E||Z) after this both these curve increases slowly and become constant after 40 eV.

The absorption spectra are depicted in Fig. 3(d). The absorption in nearly zero till 2.00 eV for E∥X, and 3.88 eV for E∥Z. Although in the case of E∥Z, curve have some small peaks at 6.25 eV, 9.19 eV and 12.97 eV, that means some absorption is also possible at these corresponding photon energies. The maximum peak of absorption lies at 8.72 eV for E∥X, and at 19.47 eV for E∥Z, both energies are coming at ultraviolet (UV) of electromagnetic spectrum. It ensures that material have strong ability to absorb UV radiation.
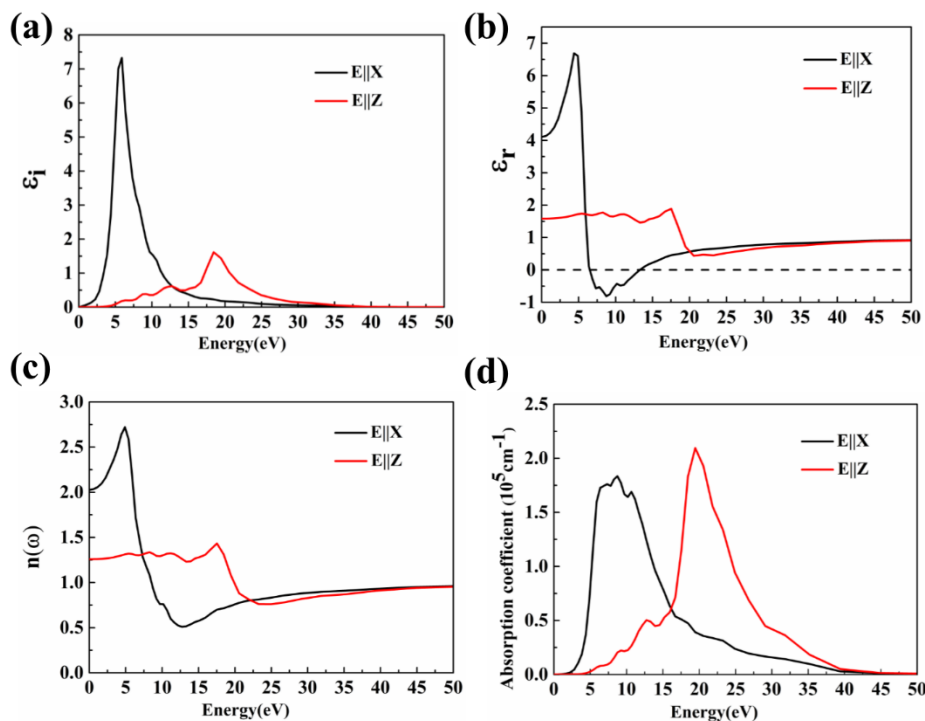

Figure 3 The optical properties (a) imaginary part of dielectric function (b) real part of dielectric function (c) refractive index (d) absorption coefficent of BSe (2H) monolayer.

Summary

We examined the structural, electronic, and optical properties of BSe (2H) monolayer by using DFT framework. The results show that BSe (H) is an indirect 2.62 eV band gap. The maximum absorption peaks observed at 8.72 eV (E∥X) and 19.72 eV (E∥Z), which lies in UV region. According to these theoretical results, the 2D BSe (2H) monolayer is viable UV absorption candidate.

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