



Theoretical investigation of electronic and optical properties of zinc blende structure of beryllium sulphide, BeS

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ABSTRACT

A theoretical study of electronic and optical properties of zinc blende structure of BeS is presented by applying the full-potential linearized augmented plane wave (FP-LAPW) method within density-functional theory (DFT) as implemented in WIEN2k code. Our results are in agreement with previous theoretical and experimental studies on this important semiconductor compound. For the optical calculations, the dipole approximation is used. The imaginary part of dielectric function is calculated in momentum representation, which requires matrix elements of the momentum p between occupied and unoccupied states. The microscopic origin of the main features in the optical spectra is identified and also the factors responsible for most of the optical absorption.

Key words: BeS; FP-LAPW; band structure; optical property; WIEN2k.

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INTRODUCTION

The II–VI semiconductors compounds have been extensively studied in recent years because of their scientific and technology interests. They are used in the fabrication of light-emitting devices that are employed in optical processing, detection systems for environmental pollution and color-displaying modules. In particular, the

beryllium chalcogenides BeS, BeSe and BeTe are the II–VI compounds that crystallize in the four-fold coordinated zinc blende (B3) structure at low pressure. In fact, probably as a result of their very high toxic nature only few experimental studies¹ have been performed on these compounds but more theoretical studies of these compounds are available in the literature.²⁻¹³ Theoretical calculation of the optical and electronic properties of BeX (X = Te, Se and S) compounds were performed by Stukel² using a first-principle self-consistent orthogonalized-

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plane wave (OPW). The calculated dielectric functions were not compared with the experimental data because no data were available at that time. A few non-relativistic local density approximation (LDA) calculations of the structural, electronic and optical properties have been performed for beryllium monochalcogenides.^{3,4} Fleszar and Hanke⁵ have calculated electronic excitations in BeX using the many-body Green's functions technique (GW) and have given a detailed discussion of LDA versus GW. Hassan and Akbarzadeh⁶ have present detail calculation of the band structure using more advanced Engel Vosko's GGA (EV-GGA) formalism. Imad Khan *et al.*⁷ have calculated electronic and optical properties of mixed Be-chalcogenides with the FP-LAPW method using a recently developed modified Beck and Johnson potential. The structural and electronic properties have also been theoretically investigated using the tight-binding linear muffin-tin orbital method (TB-LMTO).¹²

The aim of this paper is to give a comparative and complementary study of electronic properties to both experimental and other theoretical works by using FP-LAPW method as well as optical studies for BeS.

METHOD

We calculated the optical properties of BeS using the FPLAPW method¹⁴ as implemented in the WIEN2K package.¹⁵ We choose the exchange-correlation potential parameterized by Perdew *et al.*¹⁶ which is derived by using the generalized gradient approximation (GGA). In the FPLAPW method, a basis set is obtained by dividing the unit cell into non-overlapping atomic spheres (centered on the atomic sites) and an interstitial region. Inside the atomic sphere, a linear combination of radial function times spherical harmonic is used, and in the interstitial region a plane wave expansion is augmented by an atomic like function in every atomic sphere. This method yields accurate energy eigenvalues and wavefunctions, therefore appropriate for calculating the electronic and

optical properties of crystalline solids. We have chosen sphere radii of 1.8 Å for Be and 2.8 Å for S. For our calculation, we used lattice parameters $a = 4.8630$ Å for BeS.¹⁷ The values of $K_{\text{max}} \times R_{\text{MT}} = 7.0$ (where R_{MT} is the atomic sphere radius and K_{max} is the interstitial plane wave cut-off), In the atomic region, the basis set consists of spherical harmonics with angular quantum number $l = 10$ and a non spherical contribution with $l = 4$ are kept constant throughout the calculations. The self-consistent iterations are considered to be converged when the total energy of the system are stable within 10^{-5} Ry. The semiconducting beryllium sulphide crystallized in the zinc blende structure. The space group is F-43 m. The Be atom is located at the origin and the S atom is located at (1/4, 1/4, 1/4). In a cubic unit cell only one component of the dielectric function has to be calculated, i.e. ϵ_{xx} , written as

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega) \quad (1)$$

describes the optical response of the system at all photon energies $E = \hbar\omega$. The imaginary part of the dielectric function $\epsilon_2(\omega)$ is given by¹⁸

$$\epsilon_2(\omega) = \left(\frac{4\pi e^2}{m^2 \omega^2} \right) \sum_{ij} \langle i | M | j \rangle^2 f_i (1 - f_j) \times \delta(E_f - E_i - \omega) d^3k \quad (2)$$

where M is the dipole matrix element, i and j are the initial and final states, respectively, f_i is the Fermi distribution function for the i^{th} state. E_i is the energy of electron in the i^{th} states. The real part of the dielectric function $\epsilon_1(\omega)$ can be extracted from the imaginary part of the dielectric function $\epsilon_2(\omega)$ by using the Kramers-Kronig relation¹⁹

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{\omega' \epsilon_2(\omega')}{(\omega'^2 - \omega^2)} d\omega' \quad (3)$$

where P implies the principal value of the integral.

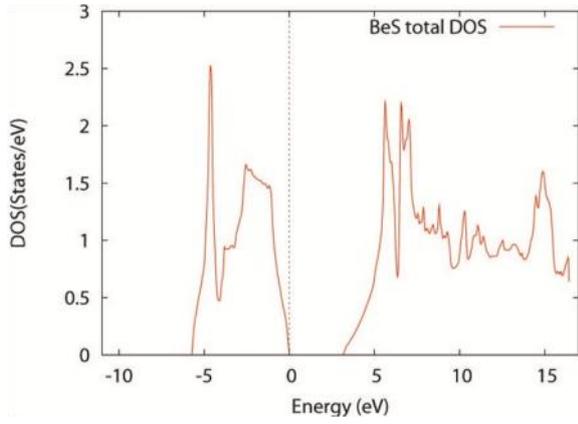


Figure 1. Total density of states for ZB BeS.

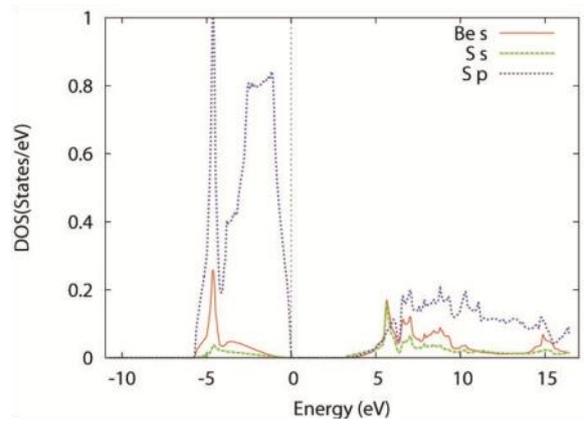


Figure 2. Partial density of states for ZB BeS.

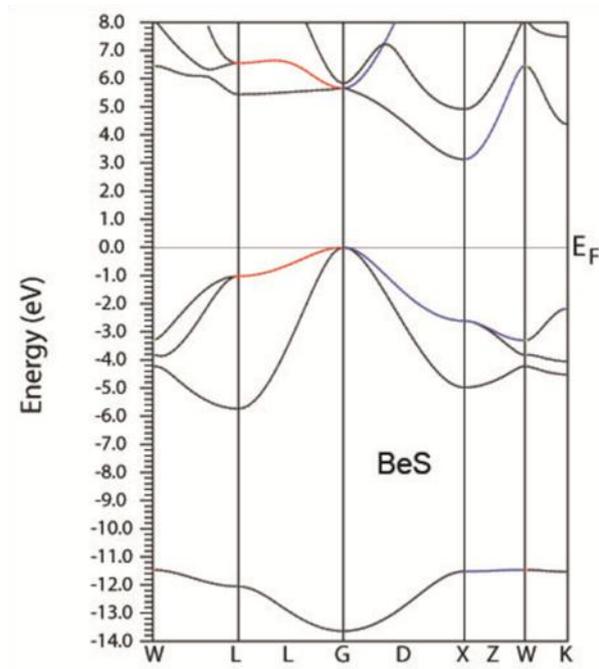


Figure 3. Band structure for BeS.

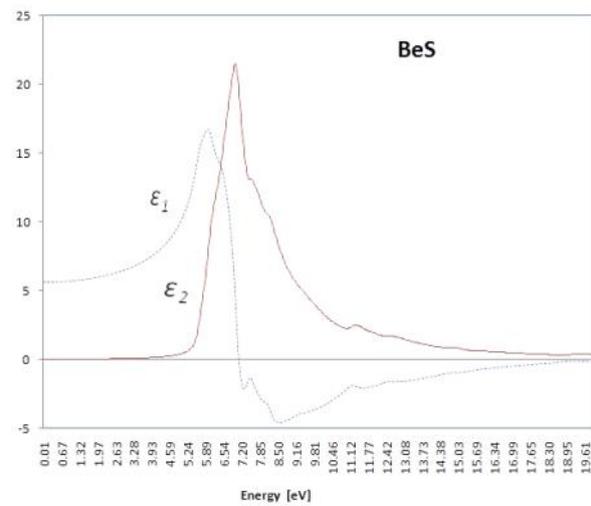


Figure 4. Real and imaginary part of dielectric function for BeS.

Table 1. Our calculated energy band gap values and the experimental and theoretical band gap (all values are in eV).

System study	Expt. Band gap	Theoretical Band gap				Present work GGA
		OPW	TB-LMTO	EV	GGA	
BeS	>5.5 ^a	4.17 ^b	3.78 ^c	4.23 ^d , 4.26 ^f , 4.241 ^g , 4.247 ^h	3.12 ^d , 4.20 ^e , 3.14 ^f , 3.141 ^g , 3.148 ^h , 2.911 ⁱ	3.12

^aRef. 1, ^bRef. 2, ^cRef. 12, ^dRef. 6, ^eRef. 7, ^fRef. 8, ^gRef. 9, ^hRef. 10, ⁱRef. 11.

RESULTS AND DISCUSSIONS

Electronic properties

For zinc blende structured of BeS, the calculated total density of states, the partial density of states and band structures are illustrated in Figures 1, 2 and 3. The valence band maximum (VBM) occurs at the Γ point and conduction band minimum (CBM) at the X point resulting in an indirect gap in agreement with experiment and previous theoretical work.¹⁻¹³ The lowest-lying band shown in the graph arises mainly from the chalcogen valence s states and the upper valence bands arises from the chalcogen valence p states with the top occurring at the Γ point. The conduction band arises mainly from the $2s$ -Be states with the minimum energy occurring at X -points.

The band gap of semiconductor BeS in the tetragonal phase as calculated by using the FP-LAPW method and using GGA approximation was found to be 3.12 eV. The important features of the band structure are given in Table 1. It is clearly seen that the band gap obtained by GGA are lower than the corresponding experimental values and results obtained from OPW and EV-GGA and not far from the results obtained by the TB-LMTO methods with the same exchange correlation approximation. This underestimation of the band gap is mainly due to the fact that the simple forms of GGA are not sufficiently flexible to accurately reproduce both exchange correlation energy and its charge derivative.

Optical properties

The determination of the optical properties of a compound in the spectral range above its band gap plays an important role in the understanding of the nature of that material and also gives a clear picture of its applications in optoelectronic devices. The detailed variation of real, $\epsilon_1(\omega)$ and imaginary $\epsilon_2(\omega)$ parts of the dielectric function for BeS with photon energy are shown in Figure 4. The $\epsilon_1(\omega)$ spectra appears at the same energy as a peak in the corresponding $\epsilon_2(\omega)$ spectra. Metallic reflectance characteristics are exhibited in the range of $\epsilon_1(\omega) < 0$. The peak of the imaginary part of the dielectric function is related to the electron excitation. It is clear from the figure that $\epsilon_2(\omega)$ shows single peak at 6.95 eV for BeS. The peaks are primarily due to transitions between valence bands and conduction bands above the Fermi energy along the symmetry lines Γ - X direction. We compare our calculated $\epsilon_2(\omega)$ with the previous theoretical calculations^{4,9,13} and agreement is found.

CONCLUSIONS

We present the electronic and optical properties of Zinc blende structure of BeS using generalized gradient approximation (GGA) within the FP-LAPW method. We found that the ZB structured BeS has indirect gap which is induced by the (Γ - X) transition with its value being 3.12 eV. We compare our calculated $\epsilon_2(\omega)$ with the previous theoretical calculations^{4,9,13} and agreement is found. The band calculations are com-

parable very well to available measurements. In addition, we revealed behaviours of TDOS and PDOS of the ZB BeS. The obtained optical parameters suggest that the strong absorption spectrum appears mostly in the ultra-violet region, and the optical absorption decreases with photon energy in the high energy range.

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