



Study of electronic and optical properties of lead telluride (PbTe) by using FP-LAPW method

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ABSTRACT

A theoretical study of electronic and optical properties of PbTe using the full-potential augmented plane waves (FP-LAPW) within density-functional theory (DFT) was presented as implemented in WIEN2k code. We adopted the dipole approximation in our optical calculations. The dielectric function was calculated in the momentum representation, which requires matrix elements of the momentum p between occupied and unoccupied states. We identified the microscopic origin of the main features in the optical spectra and find the factors responsible for most of the optical absorption in this system.

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

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INTRODUCTION

The semiconductor (IV-VI) PbTe, also known as lead salt, has been the subject of a vast amount of theoretical and experimental work during the past decades, motivated in parts by its technological usefulness, but also by their unusual interesting physical properties among semiconductors. The lead salt finds application in infrared detectors, in light emitting devices, as infrared lasers in fibre optics, as thermoelectric materials, in solar

energy panels, and in window coatings.¹⁻⁴

METHOD

The calculations reported here were performed within the generalized gradient approximation to the density functional theory as implemented in the WIEN2k computer code,⁵ using the full potential linearized augmented plane wave (FP-LAPW) method. In the full potential schemes, both the potential and charge density are expanded into lattice harmonics (inside each atomic sphere)

$$\sum_{LM} V_{LM}(r) Y_{LM}(r)$$

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and as a Fourier series (in the interstitial region):

$$\sum_K V_K e^{i\vec{K}\cdot\vec{r}}$$

Thus, their form is completely general so that such a scheme is termed full-potential calculation. In the FP-LAPW method, the unit cell is divided into non-overlapping atomic spheres and an interstitial region. Lead telluride is stable in rock-salt structure and have direct minimum energy band gap at the L symmetry point in the Brillouin Zone (BZ). For our calculation, we used lattice parameters $a = 6.54 \text{ \AA}$, which was found out from volume optimization with the optimized wave vector $k = 4000$ and atomic sphere radii 3.0 \AA and 2.8 \AA , respectively, for Pb and Te. We use $R_{\text{MT}} \times K_{\text{max}} = 7$ to determine the matrix size, where K_{max} is the plane-wave cut off and R_{MT} is the muffin tin sphere radii. In the atomic region, the basis set consists of spherical harmonics with angular quantum number $l = 10$ and a non spherical contribution with $l = 4$. We choose the exchange-correlation potential parameterized by Perdew *et al.*,⁶ which is derived by using the generalized gradient approximation (GGA). The self-consistent iterations are considered to be converged when the total energy of the system are stable within 10^{-3} mRy .

In our optical calculations, we adopted the dipole approximation, i.e. the momentum transfer from the initial state to the final state was neglected. The dielectric function was calculated in the momentum representation, which requires matrix elements of the momentum p between occupied and unoccupied states. Thus, the components of the imaginary, or absorptive part of the dielectric function, $\epsilon_2^{ij}(\omega)$ was calculated by using⁷ the relation

$$\epsilon_2^{ij}(\omega) = \frac{4\pi^2 e^2}{Vm^2 \omega^2} \times \sum_{k m \sigma} \langle k n \sigma | p_i | k n' \sigma \rangle \langle k n' \sigma | p_j | k n \sigma \rangle$$

$$\times f_{k n} (1 - f_{k n'}) \delta(E_{k n'} - E_{k n} - \hbar\omega) \quad (1)$$

where e and m is the electron charge and mass, respectively, ω is the frequency of the incoming electromagnetic radiation, V is the volume of the unit cell, $(p_x, p_y, p_z) = p$ is the momentum operator $|k n \sigma\rangle$ the crystal wave function, corresponding to eigen value $E_{k n}$ with crystal momentum k and spin σ . Finally, $f_{k n}$ is the Fermi distribution function ensuring that only transitions from occupied to unoccupied states are counted, and $\delta(E_{k n'} - E_{k n} - \hbar\omega)$ is the condition for total energy conservation. The real part (ϵ_1) can be obtained from the imaginary part (ϵ_2) by using the Kramers-Kronig dispersion relation.

RESULTS AND DISCUSSION

Band structure and bonding mechanism

The total state density of PbTe is shown in the Figure 1. As seen in the Figure, there is a narrow peak centered at around -11 eV. The partial states are shown Figures 2(a) & 2(b). It is also seen that just below the Fermi level, the bands are dominated by chalcogen p states, with some contribution coming from the Pb-6p states. In the region above the Fermi level, p states also dominate. From the partial state densities, it is clear that the main bonding mechanism in PbTe is the hybridization between the Pb-6p states and chalcogen p states. The bond is both ionic and covalent in character, covalent since the Pb-6p states and chalcogen p states are strongly hybridized and degenerate over a large part of their extension, and ionic since the relative amount of Pb-6p states and chalcogen p states is different above and below Fermi level. Below the Fermi level, the chalcogen p states dominate and above Fermi level, the Pb-6p states dominate. The calculated band structures along symmetry lines L, Γ , X, W, are displayed in Figure 3. Experimentally, it is well known that PbTe have a narrow band gap at the L

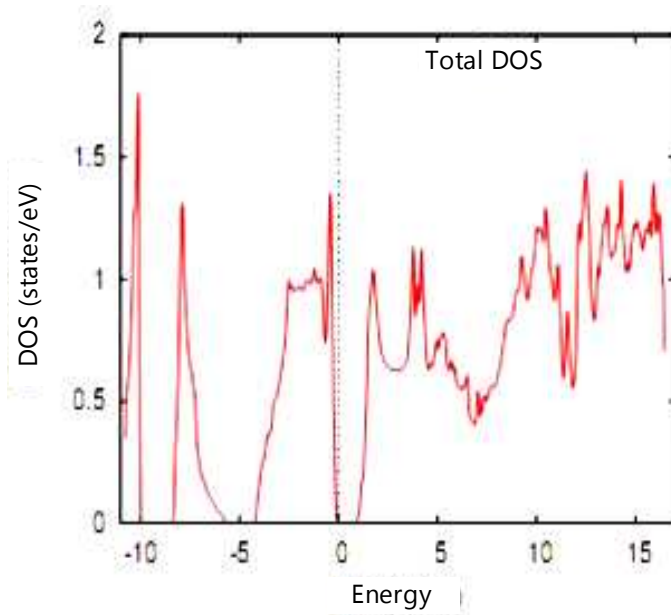


Figure 1. Total DOS (in scales per electron volt) for PbTe. The Fermi energy is at zero.

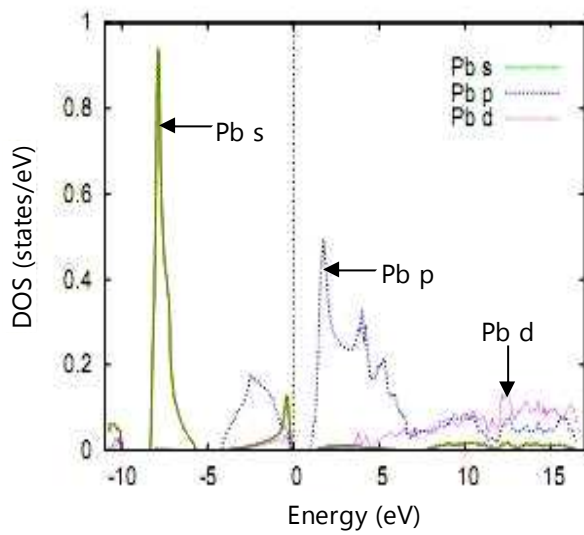


Figure 2(a). Partial DOS for Pb.

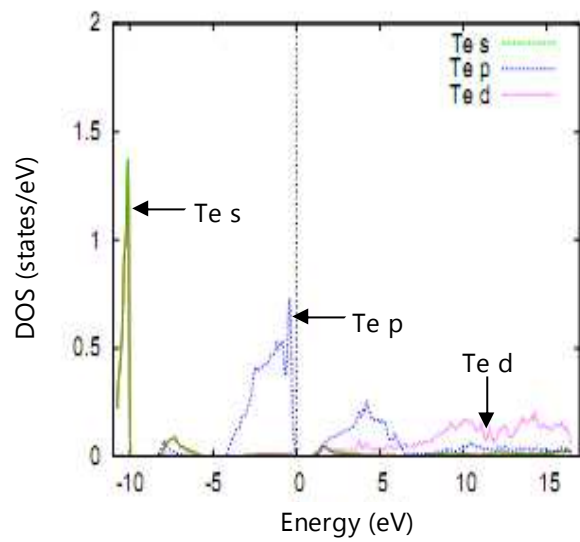


Figure 2(b). Partial DOS for Te.

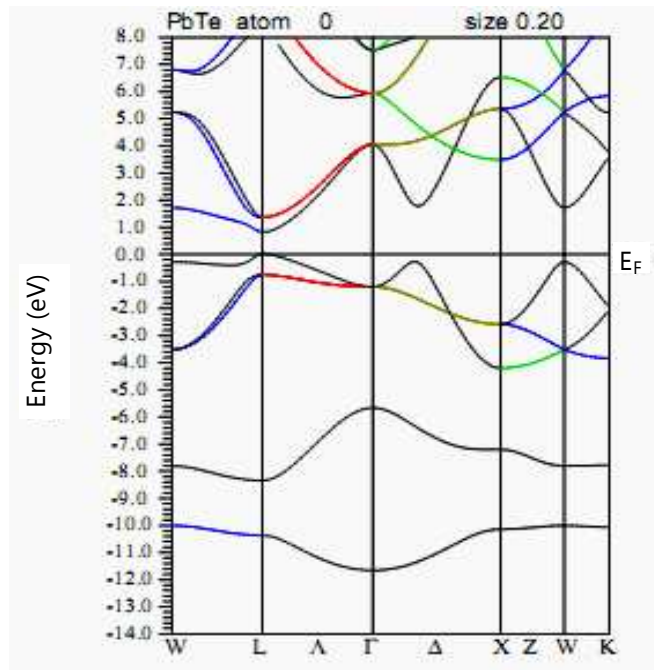


Figure 3. Band structure of PbTe along high symmetry direction in the Brillouin zone. The Fermi energy is at zero.

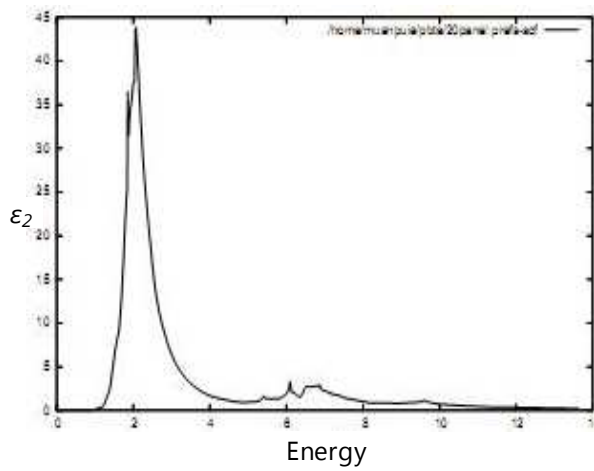


Figure 4. Calculated absorptive part of the

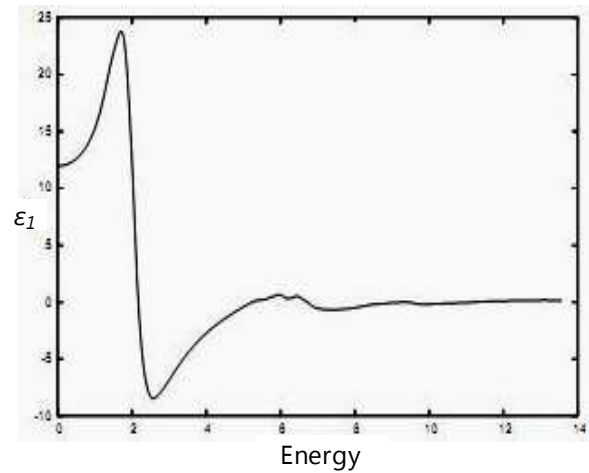


Figure 5. Calculated dispersive part of the

point. We also find energy gap of around 0.70 eV at the L point. Our calculated value of Fermi energy is 0.328 eV.

The absorptive part of the dielectric function ϵ_2 is shown in Figure 4. The main feature is a broad peak with maximum at around 2 eV. The peak reproduced in our calculation, are the general form of the spectra. The trends in ϵ_2 may be linked to the trends observed in the DOS and band structures. Our optical calculation shows that transitions between highest lying valence band (HVB) and lowest lying conduction band (LCB) account for almost all structure in optical spectra at energy below 6 eV. From the partial state densities in Figures 2(a) and 2(b), it is obvious that the p states play a major role in these optical transitions, both as initial and final states. Of the s states, the Pb state primarily serves as initial state, whereas the chalcogen state is mostly final state. The lead and chalcogen d states are primarily final states.

Next, we considered the dispersive part of the dielectric function ϵ_1 as shown in Figure 5. The calculated spectra have been obtained by Kramers-Kronig relation. The main feature is shoulder at lower energy with a steep decrease at around 2 eV, after which ϵ_1 becomes negative, a minimum and then a slow increase toward zero at higher energy. All these features show satisfactory result with the experimental spectra.⁸

CONCLUSIONS

In this paper, we report calculations of the energy bands, density of states and optical properties of PbTe using FP-LAPW method. We also identified the microscopic origin of the main features in the optical spectra and found that transitions between highest lying valence band (HVB) and lowest lying conduction band (LCB) are responsible most of the optical absorption in PbTe.

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