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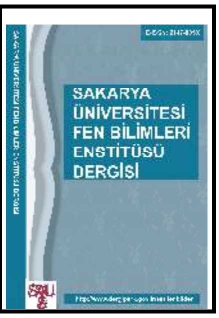

A first-principles ıinvestigation on a Half-Heusler liscpb semiconductor

Yeşim Mogulkoc*[1] and Yasemin Ciftci[2]

ABSTRACT

A first-principles study of structural, elastic, electronic, vibrational, thermodynamic and optical properties of a half-Heusler (HH) LiScPb semiconductor has been reported using the plane-wave pseudo-potential technique based on density functional theory (DFT). The elastic properties are represented using second-order elastic constants. The electronic band structure calculations are obtained with partial density of states. Optical properties of HH-LiScPb semiconductor are also investigated and related parameters such as refraction index, extinction coefficient, reflectivity and loss function are determined using dielectric functions in this study. Phonon calculations have been taken into account to evaluate the stability of half-Heusler (HH) LiScPb semiconductor. Also, the system's free energy, entropy and heat capacity were investigated under increasing temperature values.

Keywords: First-principles, half-Heusler, elastic properties, electronic properties, LiScPb

Yarı-Heusler LiScPb yarıiletkeni üzerine bir ilk ilkesel araştırma

ÖZ

Bir ilk-ilkesel çalışması olan yarı-Heusler (HH) LiScPb yarıiletkeninin yapısal, elastik, elektronik, titreşimsel, termodinamik ve optik özellikleri yoğunluk fonksiyoneli teorisine dayanan düzlem dalga-pseudo potansiyel tekniği kullanılarak rapor edilmiştir. Elastik özellikler ikinci mertebeden elastik sabitleri kullanılarak sunulmuştur. Elektronik bant yapısı hesaplamaları kısmi durum yoğunlukları ile elde edilmiştir. Yarı-Heusler (HH) LiScPb yarıiletkeninin optiksel özellikleri araştırılmıştır ve bu çalışmada kırılma indisi, sönüm katsayısı, yansıma ve kayıp fonksiyonu dielektrik fonksiyonları kullanılarak belirlenmiştir. Yarı-Heusler (HH) LiScPb yarıiletkeninin kararlılığını değerlendirmek için fonon hesaplamaları dikkate alınmıştır. Ayrıca, sistemin serbest enerjisi, entropisi ve ısı sıcaklığı artan sıcaklık değerleri altında araştırılmıştır.

Anahtar Kelimeler: İlk-ilkesel, yarı-Heusler, elastik özellikler, elektronik özellikler, LiScPb

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1. INTRODUCTION

Half-Heusler (HH) compounds have been attracted valuable interests in promising new semiconducting technology. The investigations on HH semiconductors are novel materials for the improvement of these types of technological materials. Generally, half-Heusler compounds XYZ crystallize in a non-centrosymmetric structure corresponding to the space group F 3m (space number: 216) [1]. In last years, the HH compounds earned reputation due to their potential applications, such as thermoelectrics, green energy-related fields and spintronics [2]. The temperature dependence of electrical conductivity, Seebeck coefficient, Hall coefficient, and thermal conductivity of Nb-doped MNiSn (M = Ti, Zr) half-Heusler compounds were investigated at different temperature, ranging from room temperature to 1000 K by Muta et al. [3]. Recent progress and advances in the half-Heusler compounds are briefly reviewed by Xie and his friends [4]. Kieven and Klenk present their first principles calculations results in order to find potential of HH materials to use in optoelectronic devices [5]. In addition to, there are some remarkable studies about topological insulators. To exemplify, Xiao and his friends [6] explore the feasibility of converting ternary half-Heusler compounds into a new class of three-dimensional topological insulators. The half-Heusler compound LiScPb is one of the most interesting HH compound to investigate due to its convenient elastic parameters, electronic, optical, vibrational and thermodynamic properties. Preferred configurations with semiconductor materials are compared for the different half-Heusler compounds by Gruhn [7]. The analysis of lattice parameters, band gaps and static dielectric constants of half-Heusler compounds at ambient pressure are investigated and demonstrated as new candidates for the optoelectronic devices by Mehnane et al. [8]. The structural, electronic and optical properties of half-Heusler compounds of I-II-V and I-III-IV types using first principles calculations based on the density functional theory by Kacimi et al. [9]. Here, we have investigated, presented and compared the structural, elastic, electronic, optical, vibrational and thermodynamic properties of half-Heusler LiScPb semiconductor. The paper is organized as follows: in Sec. II, computational model and methods are given. Results for the preferred crystal structure are separately presented in Sec. III for each physical properties of the system.

2. MODEL AND METHOD

The first-principles calculations are performed using density functional theory within the Perdew-Burke-Ernzerhof (PBE) parametrization of the generalized gradient approximation (GGA) [12, 13] as implemented in the Vienna Ab-initio Simulation Package (VASP) [10-13]. The plane wave based pseudo-potential method has been used for the total energy calculations. The electron-ion interaction and the exchange correlation energy were described under the Projector Augmented Wave (PAW) method and the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) scheme, respectively [12-13]. For the plane-wave basis set, the kinetic energy cutoff is taken to be 700 eV. Calculations have been performed to ensure convergence of the total energy in terms of the cutoff energy and k-points. The numerical integration of Brillouin zone for optimization, elastic and optical properties is applied using a 15x15x15 Monkhorst-Pack k-points sampling procedure for HH-LiScPb semiconductor while 42x42x42 k-points for band structure and 20x20x20 k-points for partial density of states are employed. Convergence test demonstrated that the values of the k-point and the cutoff energy were selected in the range that guarantees the convergence of the total energy. The convergence criterion for energy is set to 10^{-7} eV between two consecutive steps in the self-consistent field calculations. The atomic positions are relaxed until the Hellmann– Feynman forces are less than 10^{-5} eV/Å. Pressures on the lattice unit cell are decreased to values less than 1.0 kbar.

3. RESULTS AND DISCUSSION

3.1. Structural and Elastic Properties

The half-Heusler compounds are composed with ternary XYZ has a 1:1:1 stoichiometry, its space group is $\boldsymbol{F\bar{4}3m}$ and Pearson symbol is C1_b. The half-Heusler compounds have eight valance electrons, including a large number of semiconductors with energy gaps vary in a wide range [16].

The crystal structure of LiScPb half-Heusler semiconductor that has face-centered-cubic lattices with Pb is sitting at the unique site as shown in Figure 1 [17]. It can be regarded as a hybrid HH compound of LiSc with the rock-salt structure, and LiPb and PbSc with the zinc blende structures.

We have studied the structural and elastic properties in the framework of Density Functional Theory (DFT). The present lattice constant is estimated to be 6.789Å for LiScPb HH compound. The calculated present lattice constant is good agreement with the other numerical study [18] that it has 6.708Å. These fractionations may arise from the using of GGA and Local Density Approximations (LDA) with different ab-initio codes and methods.

Taking the optimized structure as a reference, a series of constant volume structural optimizations have been proved in order to obtain energy versus volume changes that allow the determination of the equilibrium volume and the bulk modulus by fitting these data to the Murnaghan equation of states (eos), appropriate for crystals at ambient pressure values [19].

The elastic properties have a crucial role in providing valuable information about the binding characteristic between atomic planes. In the framework of our calculations of elastic properties, the second-order elastic constants (C_{ij}) are calculated using by “stress-strain method” [20, 21] and these elastic constants are evaluated with respect to Born’s stability criteria that should be satisfied for the stability conditions of crystal lattice [22]. Known and substantial conditions for mechanical stability of cubic crystals are as follow [23]: $C_{11}>0$, $C_{11}-C_{12}>0$, $C_{44}>0$, $C_{11}+2C_{12}>0$ and $C_{12}<B<C_{11}$. According to Born’s stability criteria, the half-Heusler compound LiScPb in half Heusler structure is mechanically stable at zero pressure.

The bulk modulus B is the resistance of a material against volume variation of the system. Our bulk modulus is calculated as 37.39 GPa at zero pressure. Comparing with reference [18] the modulus is found as 41.67 GPa calculated using by LDA but still very good convenient value (see Table 1).

For cubic materials, the shear modulus G is related to the second-order elastic constants by the relation (1) [24]. Calculated shear modulus is given in Table 1. To compare with the other reference is quite convenient using by both approximations theoretically. The Zener anisotropy parameter (Z) is also related to the elastic parameters by the relation (2) [24]. If $Z<1$, the material is stiffest along <100> cube axis, while Z>1 it is stiffest along <111> body diagonals [24]. Taken to account attention to our calculated and references values it could be acceptable situation for $Z>1$ it is stiffest along <111> body diagonals.

Kleinman parameter that describes the relative positions of the cation and anion sublattices under volume conserving strain distortions for which positions are not fixed by symmetry [25]. Kleinman parameter is defined as relation (3) [26]. The evaluated Kleinman parameter is found as 0.59 at zero pressure for the half-Heusler LiScPb compound.

3.2. Electronic and Optical Properties

The electronic structure of half-Heusler LiScPb semiconductor is investigated by the electronic band structures with total and partial density of states that are depicted in Figures 2 and 3 at equilibrium lattice constant.

The calculated band structure of half-Heusler LiScPb compound along the high symmetry directions of the Brillouin zone is shown in Figure 2. It can be seen that LiScPb has a indirect band gap material with a band gap of 0.702 eV at zero pressure for present study while 0.510 eV for Ref. [18] with LDA. According to Figure 2, the top of valance band is located at Γ-point and the bottom of the conduct band is located at X-point are clearly observed. The Fermi energy is set to zero. The total density of states of half-Heusler LiScPb compound is also shown in Figure 2.

The density of states (DOS) of a system describes the number of states at each energy level, which is available to be occupied in condensed matter physics. We have presented the total density of states and partial density of states (PDOS) of half-Heusler LiScPb compound in Figure 3. As it is clearly illustrated in Figure 3, under the conventional GGA-PBE model, the contribution to the lower valance bands are mainly Li-p states (located at nearly -1 eV), the middle valance bands are mainly the Sc-d states (located at -1 ~ -1.5 eV) and the upper valance bands are dominated by Pb-p states (located at -2 – 0 eV). The conductions bands are mainly from Sc-d states and Pb-d states, partially Li-p states. Sc-d states have a maximum at around 2 eV. The half-Heusler LiScPb compound has a semiconducting behavior due to the fact that it has band gap.

The optical properties of half-Heusler LiScPb semiconductor are also determined and discussed due the fact that it is demonstrated as an optoelectronic device in technological studies. The optical properties of a solid material are usually described by the complex dielectric function by the $\varepsilon(\omega)=\varepsilon_1(\omega)+i\varepsilon_2(\omega)$ relation. The complex dielectric function characterizes the linear response of the material to an electromagnetic radiation. The imaginary part of dielectric function $\varepsilon_2(\omega)$ represents the optical absorption in the crystal. $\varepsilon_2(\omega)$ can be calculated using by the momentum matrix elements between the occupied and unoccupied wavefunctions. The real part of dielectric function $\varepsilon_1(\omega)$ is calculated using Kramers–Kroning relations. The real part of dielectric function is found as the relation (4) in where M is the principle value of the integral.

The imaginary part of the dielectric function is calculated from the matrix elements as relation (5). In the formula (5), V is the volume of the unit cell, e is the electron charge, m is its mass, $|kn\rangle$ is the wave function of the crystal, $f(kn)$ is the Fermi-Dirac function distribution, n' is the incident photon energy, n refers the unoccupied wave functions and n' refers the occupied wave functions.

Figure 4 illustrates the calculated dielectric function of the half-Heusler LiScPb compound. It can be seen that the imaginary spectrum of $\varepsilon(\omega)$ has a prominent absorption peak, located at the photon energy of nearly 2.5 eV.

The expressions of optical properties using by dielectric functions, refractive index $n(\omega)$, extinction coefficient $k(\omega)$, reflectivity $R(\omega)$ and energy loss function $L(\omega)$ are given respectively as relations (6-9) [27, 28]. Using these relations, the determined optical parameters are plotted in Figure 5.

According to the dispersion curve of refractive index at $\omega=0$, $n(\omega)$ is found to be 4.6 and the extinction coefficient ($k(\omega)$) is estimated as 5.0 as shown in Figure 5. Reflectivity has less peak values in contrast to loss function. The main peak as it is known plasmon frequency (ω_p) is evaluated in the energy loss functions $L(\omega)$ and is located at nearly 12.5 eV. For reflectivity, the main peak is observed at around 8 eV and second main peak is at around 32 eV.

3.3. Vibrational and Thermodynamic Properties

Phonon plays essential roles in vibrational properties, which are basic topics dynamically in the fundamentals of materials science. The first principles phonon calculations cannot be completely emphasized. PHONOPY [29] is an open source code for phonons based calculations. It has been described dynamical properties of materials at finite temperature in this code. Here, we have demonstrated the phonon properties with related phonon dispersion curves.

The phonon dispersion curves in high symmetry directions with 24 atoms have been calculated using 2x2x2 supercell. The obtained results are illustrated in Figure 6 with partial and total density of states of half-Heusler LiScPb compound. There are three optical and six acoustic branches for this compound. As it is seen from the Figure 6, all frequency values of compound are positive and we have concluded that half-Heusler LiScPb compound is dynamically stable. Considering for this HH-compound, it is also depicted that from partial density of states, Li and Sc atoms give a huge contribution to the acoustic part of phonon branches when Pb atom gives a huge contribution to the optical branches of phonons.

After obtaining the phonon density of states (PHDOS), we calculated the thermodynamic properties of LiScPb by means of the quasi-harmonic approximation and PHONONPY package. The thermodynamic quantities have been studied based on the quasi-harmonic approach and thermal electronic excitation. By using the phonon spectra, the thermodynamic parameters such as free energy (*F*), entropy (*S*) and heat capacity (*Cv*) have been calculated as shown in Figure 7. The free energy of the system is important to get information about thermodynamics of the system which has also known as thermodynamic potential energy. Figure 7 indicates that the entropy of LiScPb increases gradually with the elevated temperature, while the free energy decreases with the increase of temperature. It can be seen from Figure 7 that the heat capacities *Cv* of LiScPb increase very rapidly and proportionally to T^3 with elevated temperature in the low temperature region, which obeys Debye's law. When the temperature is above 400K, the C_V has not been changed with temperature and approaches approximately the Dulong–Petit limit owing to the Debye model (C_V~ 73 J/(K'mol)).

4. SUMMARY AND CONCLUSION

The first-principles calculations have been carried out of the structural, elastic properties, electronic properties, optical properties, vibrational properties and thermodynamic properties of half-Heusler LiScPb compound. The obtained results have shown that the half-Heusler LiScPb compound is mechanically stable in considered structure. The mechanical stability and elasticity are also considered and presented. The electronic properties are also investigated and depicted that with partial density of states for LiScPb HH compound. Also, LiScPb has an indirect band gap material with a band gap of 0.702 eV at zero pressure. The general optical parameters are evaluated with convenient values. The refraction index, *n(ω)* is found to be 4.6. According to the vibrational properties, half-Heusler LiScPb compound has been observed dynamically stable. The free energy, entropy and the heat capacity values are also have been carried out for LiScPb HH compound. It is concluded that from the present study reveals that many physical properties of LiScPb HH compound have been evaluated.

5. FOOTNOTES, FIGURES AND TABLES

5.1. Tables and Figures

Table 1. Structural and elastic parameters for LiScPb HH-compound

LiScPb	*a* [Å]	C_{11} [GPa]	C_{12} [GPa]	C_{44} [GPa]	*B* [GPa]	*G* [GPa]	*Z* [GPa]
Present	6.789	59.95	28.11	15.82	37.39	15.92	0.99
Theory [18](LDA)	6.708	65.00	30.00	21.00	41.67	17.50	1.20

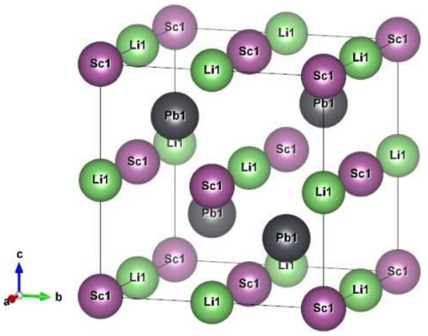

Figure 1. The crystal structure of LiScPb

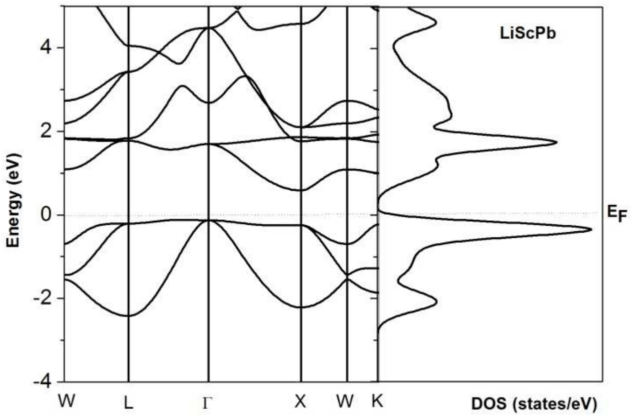

Figure 2. Electronic band structure and density of states of half-Heusler LiScPb compound

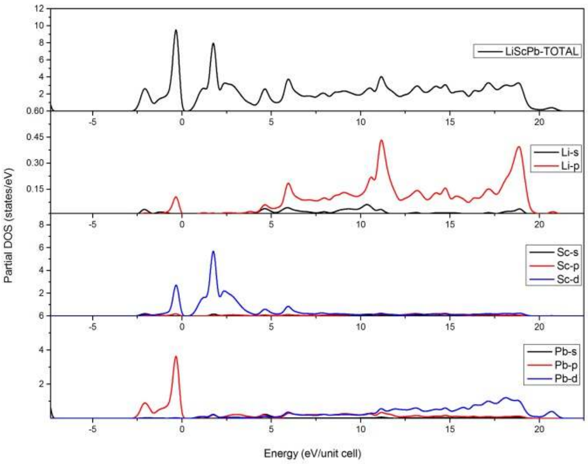

Figure 3. Partial density of states of half-Heusler LiScPb compound

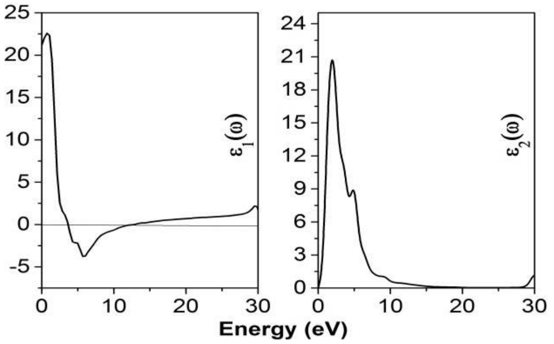

Figure 4. Real part of dielectric function (*ε₁(ω)*) and imaginer part of dielectric function (*ε₂(ω)*) of half-Heusler LiScPb compound

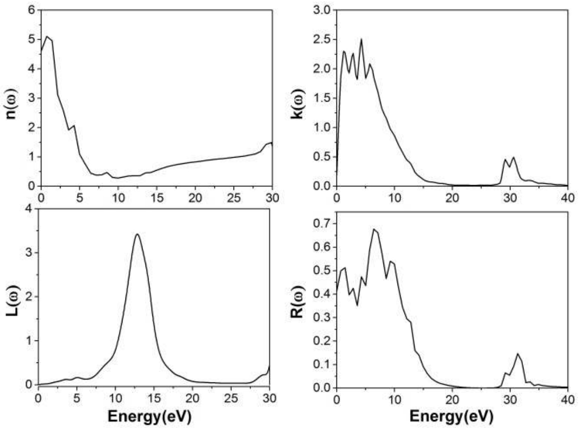

Figure 5. Refractive index *n(ω)*, extinction coefficient *k(ω)*, reflectivity *R(ω)* and energy loss function *L(ω)* of half-Heusler LiScPb compound

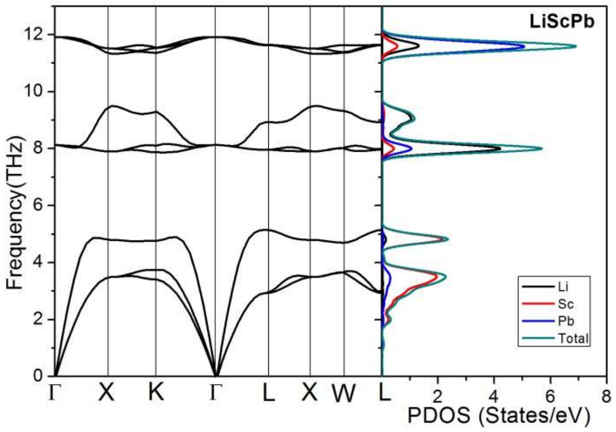

Figure 6. Phonon frequencies and partial and total density of states of half-Heusler LiScPb compound

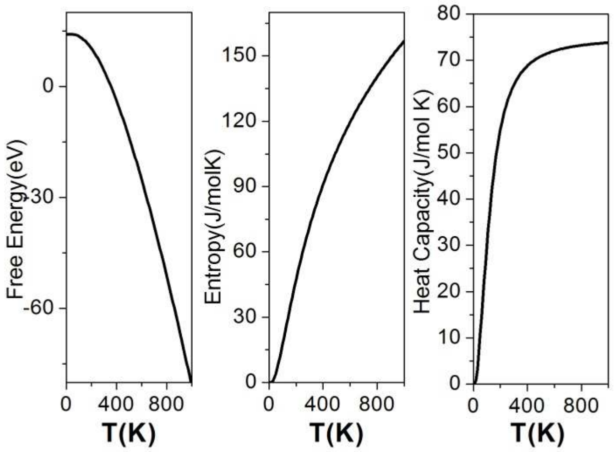

Figure 7. Thermodynamic properties of half-Heusler LiScPb compound

5.2. Formulas

All formulas are given below:

$$G = \frac{C_{11} - C_{12}}{2} \tag{1}$$

$$Z = \frac{2C_{44}}{C_{11} - C_{12}} \tag{2}$$

$$\xi = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}} \tag{3}$$

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} M \int_0^\infty \frac{\varepsilon_2(\omega')\omega'}{\omega'^2 - \omega^2} d\omega \tag{4}$$

$$\varepsilon_2(\omega) = \frac{\mathrm{Ve}^2}{2\pi\hbar \mathrm{m}^2\omega^2} \int \mathrm{d}^3\mathrm{k} \bullet \sum_{\mathrm{n,n'}} \left| \langle \mathrm{kn} | \mathrm{p} | \mathrm{kn'} \rangle^2 \right| \mathrm{f(kn)}(1 - \mathrm{f(kn')})\delta\left(\mathrm{E_{kn}} - \mathrm{E_{kn'}} - \hbar\omega\right) \tag{5}$$

$$n(\omega)=\left(\frac{\varepsilon_1(\omega)}{2}+\frac{\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}}{2}\right)^{1/2} \quad (6)$$

$$k(\omega)=\left(\frac{\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}-\varepsilon_1(\omega)}{2}\right)^{1/2} \quad (7)$$

$$R(\omega)=\left(\frac{(n(\omega)-1)^2+k(\omega)^2}{(n(\omega)+1)^2+k(\omega)^2}\right) \quad (8)$$

$$L(\omega)=\left(\frac{\varepsilon_2(\omega)}{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}\right) \quad (9)$$

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