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Tuning the optical properties through bandgap engineering in Si-doped YAuPb: *ab initio* study

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87\Abstract

In order to probe the band gap engineering to tune optical properties in YAuPb_{1-x}Si_x ($x = 0, 0.25, 0.50, 0.75$ and 1) alloys, we used all electron full-potential linearized augmented plane wave (FP-LAPW+lo) method within the frame work of the density functional theory. The optimized structural parameters were in good agreement with other theoretical and experimental results. The calculated results of elastic constant satisfy the condition for mechanical stability at each composition for cubic symmetry. In addition, the study of elastic parameters are summarized for the calculation bulk modulus, Young's modulus, shear modulus, Kleinman parameters, Poisson's ratio and Lamé's co-efficient. To predict the brittle (ductile) nature of this composition, the Cauchy pressure, Poisson's ratio and B/G ratio were also calculated. Using modified Becke and Johnson GGA, the band gap values of each composition were computed precisely. Further, it was observed that for $0.25 < x < 0.75$, band gap structure revealed a direct band gap configuration. In order to analyze the electronic structure of each composition, the total and partial densities of states have been investigated in detail. Furthermore, the investigation of

optical parameters in terms of dielectric functions revealed the potential of these alloys for optoelectronic devices.

1. Introduction

In the past couple of decades, a new emerging field in condensed matter physics is the topological insulators which are based on the realization of spin orbit coupling in electronic materials. In this field, half metallic materials gained much attention because their electrons with spin direction are metallic whereas the electrons in other directions are insulator/semiconductor. After the discovery of half metallic characteristics in NiMnSb by Groot et al. [1] by first principles, these properties were revealed in many other alloys later on. Such materials show the exotic metallic characteristics [2]. They display distinct quantum states along the edges and on the surface where electron can travel without any energy dissipation [3-5]. The topological phases of the materials can be studied by different methods. Among the different methods, Fu and Kane suggested the parity approach to probe the topological phase of the material [6]. However, this approach works only for materials having inversion symmetry. Bulk band structure is the key feature to calculate the topological in-variance [7]. The band splitting at Γ symmetry point caused by the variation in topological order is actually take place due to the band inversion. Some materials are there, which are normally insulators but when they are exposed to high pressure they show metallic like behavior.

Heusler alloys are mainly divided into two types namely full Heusler and half Heusler. Full Heusler alloys having general formula X_2YZ with space group F_{43m} and have four interpenetrating cubic sublattices [8]. Half Heusler alloys are the ternary material with general formula XYZ where X and Y are usually occupied by the transition elements while Z site by some heavy metal. The structure of half Heusler can be considered as a hybrid structure. In cubic symmetry they crystallize out as zinc blend structure [9]. These compounds gained much attention because of their variety of crystal structure, optical and transport properties [10]. Recently, researchers working in different groups used different packages to study the electronic band structures of $YAuPb$ to check its potential for topological applications [11-13]. In addition to this, Singh et al [14] investigated the thermoelectric response of the same composition using Quantum Espresso code and noticed the zero band gap of this semiconductor. However, Kandpal *et al.* [15] probed the structural parameters like lattice constant and bulk modulus and observed that this composition is quite stable.

This comprehensive literature on end compounds provide enough motivation to investigate the topological phase of half Heusler alloys and thus present work comprises the theoretical investigation of elastic, electronic and optical properties of Si substituted YAuPb alloys. These alloys have potential for optoelectronic devices which highlighted the novelty of this work.

2. Computational details

Certain lapses of distance do not let the correlations of random alloys accurate in periodic structure. For its solution, the construction of super-cell is extremely necessary. On the other hand, as the number of atoms in super-cell increases, the first-principles calculations turn to be more expensive. However, physical features largely depend on the microscopic length and local randomness to which the size of super-cell does not affect Zunger *et al.* [16]. This fact proposes the construction of special quasi-random structure (SQS) super-cells [17]. In order to find out the physical properties of YAuPb_{1-x}Si_x alloy by utilizing the compositions $x = 0.25, 0.5$ and 0.75 respectively as shown in Fig. 1.

The smallest SQS (Fig. 1) has been used in our calculations, which particularly reduces the computational times.

Fig. 1. Prototype of YAuPb_{1-x}Si_x alloys. Y is with brown, Pb is with red, Au is with yellow, and Si is with green colors.

Full-potential linear-augmented-plane-wave (FP-LAPW) method of DFT, with WIEN2k code [18], was employed for the calculations of the optical properties and electronic structure of $\text{YAuPb}_{1-x}\text{Si}_x$ alloys. The electronic exchange–correlation for structural optimization was set by Wu-Cohen Generalized Gradient Approximation (WC-GGA) whereas the self-consistent field energy tolerance is set to 10^{-4} Ryd [19]. It is reported that WC-GGA is for structural and electronic properties of materials [20]. The modified Becke–Johnson approximation (mBJ) [21] functional was brought into use for the improvement in the routine wise underestimation of the band gap by standard DFT functional in particular with the calculation of optical and electronic properties. A plane wave with cutoff $K_{\text{max}} \times R_{\text{MT}} = 8$ was utilized in converging of energy eigenvalues whereas the potentials and wave function were expanded in the interstitial regions as spherical harmonic, in the FP-LAPW calculations. Here, in plane wave expansion, K_{max} is the magnitude of the largest K vector whereas the smallest muffin-tin (MT) sphere radius is R_{MT} . The taken radius of MT sphere (R_{MT}) with the value of 2.5 a.u. is each for Si, Pb, Au, and Y respectively. However, within the atomic spheres, the selected value of angular momentum was maximum ($l_{\text{max}} = 10$) for wave function expansion. There was a Fourier expansion up to $G_{\text{max}} = 18$ in the charge density. Here the largest vector in the Fourier expansion is G_{max} . While in the irreducible part of the Brillouin zone, $12 \times 12 \times 12$ k-mesh was used to affect the Brillouin zone integration for the purpose of energy computations. For better convergence, both the number of k-points and the MT radius were varied with the selection of the value that yielded true convergence of minimum total energy. Cubic-elastic software implemented in WIEN2k [18] was employed to calculate the elastic constants of $\text{YAuPb}_{1-x}\text{Si}_x$ compounds in our study. Three independent elastic constants C_{11} , C_{12} and C_{44} are possessed by a cubic lattice. After the their computations, these constants are further employed for the evaluation of the mechanical properties of $\text{YAuPb}_{1-x}\text{Si}_x$ such as anisotropy constant (A), Kleinman parameter (ζ), Poisson's ratio (ν), Cauchy pressure (C''), Young's modulus (Y), and shear modulus (G_H), using standard relations.

3. Results and discussion

3.1. Structural properties

The structural investigations of $\text{YAuPb}_{1-x}\text{Si}_x$ alloys have been carried out by WC-GGA. The total energy optimization is done in terms of unit cell volume as mentioned in some recent reports [22, 23]. The energy optimization plots are shown in Fig. 2. The optimized lattice parameters and

bulk modulus are summarized in Table 1. In all these calculated values, the results of YAuPb and YAuSi were very close to experimental values. It is due to fact that WC-GGA approach produces lattice parameters in between the underestimated (calculated by LDA) and overestimated (calculated by GGA) results.

Fig. 2. Calculated total energy as a function of unit cell volume for YAuPb_{1-x}Si_x alloys at x = 0, 0.25, 0.50 and 0.75.

Table 1: Calculated structural parameters for $\text{YAuPb}_{1-x}\text{Si}_x$ alloys compared with experimental and other theoretical calculations.

Composition X	Lattice constant a (Å)			Bulk modulus B (GPa)		
	GGA	Other calculations	Exp.	GGA	Other calculations	Exp.
0	6.748	6.737 ^b , 6.73 ^c , 6.842 ^d	6.728 ^a	78.939	84.18 ^b , 70.6 ^d	-
0.25	6.673			86.113		
0.50	6.589			90.698		
0.75	6.495			96.457		
1	6.399	6.380 ^b		102.012	102.78 ^b	

Ref. [24]^a, Ref. [25]^b, Ref. [26]^c, Ref. [27]^d,

Fig. 3 (a & b) shows the variation of lattice parameter and bulk modulus with substitution contents (x). The lattice parameter decreased linearly with substitution of Si (see Fig. 3(a)) at the place of Pb in accordance with the Vegard's law [28,29]. In contrast to lattice parameters, bulk modulus exposed the opposite trend, which revealed that with increase of Si contents, the alloy under study became more compressible.

Fig. 3. Composition dependence of (a) lattice constant and (b) bulk modulus for $\text{YAuPb}_{1-x}\text{Si}_x$ alloys. The solid line is WC-GGA and dotted lines is Vegard's law fitting.

3.2 Elastic and Mechanical properties

The calculation of mechanical properties of any material provides useful information regarding the nature and strength of binding between nearest atoms, compressibility and anisotropy of the material [30, 31]. The elastic constant C_{11} determine the stiffness and C_{12} and C_{44} determine shape related elastic constant. The calculated second order elastic constant for $\text{YAuPb}_{1-x}\text{Si}_x$ alloys are listed in Table 2. These calculated results revealed the condition for mechanical stability for cubic symmetry, i.e. $C_{11} + 2C_{12} > 0$, $C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$ and $C_{12} < B < C_{11}$, thus these composition are mechanical stable against elastic deformation [32, 33].

Table 2: Calculated second order elastic constants (SOECs) in GPa for $\text{YAuPb}_{1-x}\text{Si}_x$ alloys.

	C_{11}	C_{12}	C_{44}	$C_{11}-C_{12}$	$B=(C_{11}+2C_{12})/3$
YAuPb	103.820	69.821	12.513	26.434	85.971
YAuPb _{0.75} Si _{0.25}	121.542	77.386	57.060	51.721	87.052
YAuPb _{0.50} Si _{0.50}	130.922	70.092	66.945	60.83	90.367
YAuPb _{0.25} Si _{0.75}	136.375	75.625	73.136	70.75	95.888
YAuSi	158.021	77.281	80.634	80.74	104.164

From these parameters one can determine strength, stability, thermo-elastic stress and toughness of the material. The calculated values of shear modulus (G_H), Young's modulus (Y), B/G ratio, Cauchy pressure (C''), Poisson's ratio (ν), Kleinman's parameter (ζ), anisotropy factor (A) and shear constant (C') are listed in Table 3. The materials response towards shear strain is determined from the shear modulus which is calculated from the Voigt shear modulus (G_V) and Reuss shear modulus (G_R) by the following relations [34-37]:

$$G_v = \frac{1}{5}(3C_{44} + C_{11} - C_{22}) \quad (1)$$

$$G_R = \frac{5(C_{11}-C_{22})C_{44}}{4C_4+3(C_{11}-C_{22})} \quad (2)$$

Where shear modulus is the arithmetic means of G_V and G_R :

i.e.

$$G_H = \frac{G_V + G_R}{2} \quad (3)$$

The high value of shear modulus (61.08 GPa) for YAuSi as compared with YAuPb (12.79) shows its high resistance towards plastic deformation. All other compositions have relatively smaller value of shear modulus which indicates their less resistive nature towards permanent change in their shape. The stiffness of any material is calculated in terms of Young's modulus which can be calculated as

$$Y = \frac{9BG_V}{3B + G_V} \quad (4)$$

Greater the value of Y, the stiffer is the material. Table 3 comprising the values of Y for all compositions convinces that YAuSi is stiffer comparatively. The brittle/ductile nature can be calculated from the ratio of bulk modulus to shear modulus (B/G) as proposed by Pugh [38]. This ratio serves as basic criteria to distinguish brittle substances from the ductile. If $B/G < 1.75$, material behavior is brittle otherwise its response is ductile towards external pressure. The calculated values of B/G confirmed the brittle nature of YAuSi. An alternate approach to determine the brittle or ductile nature of material is the Cauchy's pressure which is the difference of pressure between C_{12} and C_{44} i.e. $C'' = C_{12} - C_{44}$. Pettifor proposed that the sign ($\pm$) of C' is responsible for brittle and ductile nature of the material [39]. If the sign of C'' is negative, material is brittle otherwise ductile. From the calculated values of C' listed in table 3, it is again clear that all compositions are brittle in nature. With the help of C' values, the bonding nature of the material can also be probed. The bonding present inside the compound is ionic if C' is positive while the negative value of C' is attributed to the covalent nature of chemical bond present in the material. The most powerful tool in this regard is the Poisson's ratio, which provide the same information and can be calculated as

$$\nu = \frac{3B - Y}{6B} = \frac{1}{2} - \frac{Y}{6B} \quad (5)$$

The upper and lower limits of this ratio are 0.5 and -1.0. At the upper bound, the volume of the material remain unchanged upon increase in pressure while at the lower bound, the shape of the material remained unchanged. Frantsevish, et al. [40] used this ratio to distinguish the brittle and

ductile materials. They proposed the material is brittle, if the value of ν is less than 0.33 otherwise it is ductile [32]. Since for all $\text{YAuPb}_{1-x}\text{Si}_x$ alloys the calculated values are less than 0.33 which is another confirmation of brittle nature of the materials. In addition to this, Poisson's ratio also gives an idea about the compressibility of the material. The material is more compressible if $\nu \rightarrow 0$ [41]. Since the value of ν varies from 1-0.2, which shows that these alloys are stable against the deformation force.

When a stress force is applied, the unfixed positions of cation and anion sub-lattices are usually determined using Kleinman's parameter (ζ). The lowest value of ζ (i.e. 0) indicates that material has high resistance against bond angle distortion and bond bending as well while the high value of ζ (i.e. 1) leads to high bond stretchability [42-44]. Using elastic constants, the value of ζ can be calculated as

$$\zeta = \frac{C_{11} + 8C_{22}}{7C_{11} - 2C_{22}} \quad (6)$$

The bond stretching in $\text{YAuPb}_{1-x}\text{Si}_x$ alloys is evident from the calculated values of ζ summarized in Table 3. The microcracks in the material are detected from the anisotropy of the material which can be calculated as

$$A = \frac{2C_{44}}{C_{11} - C_{22}} \quad (7)$$

The value of A for isotropic material comes out to be 1. The deviation of value of A from unity indicates that these alloys are isotropic in nature and show different properties in different directions. Other mechanical parameters include Lamé's constants (λ , μ) which determine the hardness of the material. These parameters can be calculated in terms of Young's modulus and Poisson's ratio

$$\lambda = \frac{Y\nu}{(1+\nu)(1-2\nu)} \quad (8)$$

$$\mu = \frac{Y}{2(1+\nu)} \quad (9)$$

Here λ and μ determine the compressibility and shear stiffness of the material [45]. The values of these Lamé's constants are listed in table 3. This table interestingly revealed that the second Lamé's constant is same as that of Voigt's shear modulus (G_V). However, for isotropic materials, $\lambda = \mu = C'$ and $\mu = C'$. Since the alloys under study are highly anisotropic, thus they do not satisfy the isotropic condition i.e. $\lambda = C_{12}$ and $\mu = C'$. Tetragonal shear modulus is a necessary criterion to determine the mechanical stability and can be calculated as

$$C' = \frac{C_{11} - C_{12}}{2} \quad (10)$$

The positive values of shear modulus confirmed the mechanical stability of these alloys.

Table 3: The calculated value of Voigt's shear modulus G_v , Reuss's shear modulus G_R , Hill's shear modulus G_H , B/G ratio, Cauchy Pressure (C''), Poisson's ratio (ν), Kleinman Parameter (ζ), Anisotropy constant (A), Lames Coefficient (λ and μ), and Shear Constant (C').

	YAuPb	YAuPb _{0.75} Si _{0.25}	YAuPb _{0.5} Si _{0.50}	YAuPb _{0.25} Si _{0.75}	YAuSi
G_v	12.794	44.580	52.333	56.031	64.528
G_R	12.785	38.486	45.220	46.788	57.638
G_H	12.79	41.533	48.776	51.410	61.083
Y	36.574	114.241	131.596	140.687	160.460
B/G	6.73943	2.096	1.852	1.864	1.70576
C''	64.873	12.761	3.147	2.489	-3.353
ν	0.429	0.281	0.257	0.255	0.243
ζ	1.263	0.956	0.891	0.922	0.815
A	0.946	2.206	2.201	2.407	1.997
λ	77.667	57.341	55.48	58.520	61.175
μ	12.794	44.580	52.333	56.031	64.528
C'	13.217	25.860	30.415	30.375	40.37

3.2. Electronic properties

The thorough understanding of band gap structure provides useful information regarding the potential of different materials optoelectronic devices. Using WC-GGA and modified becke-johnson approximation (mBJ), band structure of YAuPb_{1-x}Si_x alloys is calculated, it was observed that band gap values are in good agreement with results calculated other theoretical and experimental. Same results were observed using computationally expensive software i.e. GW or hybrid functional methods [46]. The calculated band structure using mBJ + WGGA are shown in Fig. 4 and calculated values of band gap are listed in Table 3. These structures clearly shows that

valley of conduction band and peak of valence band lie at the same Γ -point of the Brillouin zone which confirmed the direct band gap semiconducting nature of these alloys.

Table 3: Band gaps for $\text{YAuPb}_{1-x}\text{Si}_x$ alloys along Γ - Γ symmetry points with WC-GGA and mBJ function.

Composition	Band gap energy (eV)				
	GGA	mBJ	Exp.	Other calculations	
YAuPb	0	0	0 ^[24]	0 ^[27]	
YAuPb _{0.75} Si _{0.25}	0.108	0.277			
YAuPb _{0.50} Si _{0.50}	0.249	0.417			
YAuPb _{0.25} Si _{0.75}	0.250	0.422			
YAuSi	0.282	0.455			

The comparison of band gap values calculated using different codes indicated that these values are higher when mBJLDA is used as compared with WC-GGA code. This indicates the improvement of band gap structure as compared with those estimated using LDA and GGA [46, 47]. It is important to note that the effect of size of supercell on the band structure was also studied. We also calculated band structure using larger (32-atoms) ZB supercells, to probe the effect of larger number of neighboring atoms on the electronic properties of these alloys. It is observed that due to the decrease of symmetry, band gap structure show a noticeable difference with unchanged nature of direct band gap.

Fig. 4. Electronic band structures plot computed using the (a) GGA (WC) and (b) mBJ functional for $\text{YAuPb}_{1-x}\text{Si}_x$ alloys at $x=0, 0.25, 0.50, 0.75$ and 1 .

The total and partial density of states (DOS) were also plotted to have better insight of electronic properties. The participation of partial and total DOS in VB and CB are identical and their results are plotted in Fig. 5. The total DOS (TDOS) and partial DOS (PDOS) of the under study alloys for various Si contents have been plotted here. From these plots it is obvious that d-states of Y splits into t_{2g} and e_g which are plotted with p-states of Pb, Si and Au. It is noticeable that end members have significantly different energy band gaps. It is observed that p-states of Pb and Si along with p-d states of Au form the valence band while d-states of Y are responsible for the formation of conduction bands. In this ternary alloy, p and d states of Au occupy the bottom of valence band on the other hand d state of Y (t_{2g} and e_g) form the top and bottom of conduction band accordingly. However, all compositions revealed the direct band gap configuration in under study alloys.

Fig.5. TDOS of $\text{YAuPb}_{1-x}\text{Si}_x$ alloys

3.3. Optical properties

To check the potential of any material for optical activity we usually examine its electronic transition at high symmetry points in the Brillouin zone from filled energy level to unfilled energy level. The interaction of any physical system with electromagnetic field can be studied with the help of dielectric function. The degree of polarization caused by the electromagnetic waves inside the materials play important role in its optical response. The complex dielectric response is a useful tool to check its optical properties. The real and imaginary parts of dielectric constant can be calculated using the following equations [48, 49]:

$$\epsilon_{real}(\omega) = 1 + \chi + \frac{Ne^2}{\epsilon_0 m_0} \frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2} \quad (11)$$

$$\epsilon_{imaginary}(\omega) = \frac{e^2 \hbar}{\pi m^2 \omega^2} \sum \int [|M_{c,v}(k)|^2 \delta[\omega_{c,v}(k) - \omega]] d^3k \quad (12)$$

Here, $\epsilon_{\text{real}}(\omega)$ and $\epsilon_{\text{imag}}(\omega)$ are the real and imaginary parts of complex dielectric constant, $M_{c,v}(k)$ shows the moment which is associated with jumping of electron from VB to CB, and $\omega_{c,v}(k) = E_{ck} - E_{vk}$ gives the transition energy. The real part determines the energy dispersion due to the incident part while the imaginary part indicates the energy absorbed by the material. The calculated values of real and imaginary parts of the dielectric constants are listed in table 4.

Table 4: Calculated optical parameters for $\text{YAuPb}_{1-x}\text{Si}_x$ alloys with mBJ functional.

	E_g (eV)	$n(0)$	$\epsilon_1(0)$	$R(0)$	Critical points values			
					ϵ_2	K	A	σ
YAuPb	0	5.12	27.4	0.450	1.39	0.132	1.82	2.54
YAuPb _{0.75} Si _{0.25}	0.277	4.97	24.75	0.439	0.768	0.077	0.010	1.406
YAuPb _{0.50} Si _{0.50}	0.417	4.64	21.54	0.414	0.503	0.054	0.007	0.922
YAuPb _{0.25} Si _{0.75}	0.422	4.41	19.46	0.393	0.393	0.044	0.006	0.719
YAuSi	0.455	4.19	17.62	0.374	0.316	0.037	0.005	0.578

Fig.6. The calculated (a) complex refractive index, (b) absorption coefficient, (c) Optical conductivity, and (d) reflectivity of $\text{YAuPb}_{1-x}\text{Si}_x$ at $x = 0, 0.25, 0.50, 0.75$ and 1 .

It is observed that with the increase of Si contents in YAuPb, the peaks shifts towards lower photon energy and become sharper as well. The value of $\epsilon_{\text{real}}(\omega)$ for YAuPb remained positive up to 15.30 eV with peaks appeared at 1.7eV, 6.9eV, 12.86eV and 15.01eV. However, for YAuSi, only two peaks appeared at 2.91 eV and 4.21 eV and the value of $\epsilon_{\text{real}}(\omega)$ remained positive up to 4.70 eV. For intermediate compositions it remained positive up to 10.91eV, 6.19eV, 5.54eV for $x=0.25, 0.50, 0.75$, respectively. For YAuPb_{0.75}Si_{0.25} and YAuPb, two deep absorption valleys were observed in between 0.52 eV to 10.79 eV and 0.96 eV - 15.3 eV respectively. Since the value of $\epsilon_{\text{real}}(\omega)$ changes between its maximum and minimum value from where we get an idea about the propagation and damping of electromagnetic waves. The positive value of $\epsilon_{\text{real}}(\omega)$ (>0) indicates the photon propagation while its negative value confirms the damping of electromagnetic waves inside the material. However, when $\epsilon_{\text{real}}(\omega) = 0$, longitudinally polarized waves are generated. For zero frequency, it turns out to be the static dielectric constant whose value is summarized in the table 4 for different concentrations. It is observed that the value of static dielectric constant depends upon the energy band gap and can be calculated using Penn model [50]

$$\epsilon_{\text{real}}(\omega) = 1 + \left(\frac{\hbar\omega_p}{E_g} \right)^2 \quad (13)$$

Here, ω_p and E_g are the plasma frequency and band gap energy, respectively. Using this equation for the given $\epsilon_{\text{real}}(0)$, ω_p and E_g can be calculated. The calculated values of E_g listed in Table 4 shows that it increased with increase of Si contents and found maximum for YAuSi. The peak present in $\epsilon_{\text{real}}(\omega)$ spectra shifted towards lower energy region with increase of Si contents. When it becomes unity, the material shows the metallic nature.

The optical and electronic role of the material can also be probed using Refractive index measurements. It plays a very crucial role in many practical applications such as wave guides, solar cell and detectors [51]. In semiconductor physics, there are some empirical relations, which determine the relation between refractive index and energy bandgap [52, 53]. These two parameters are further used to derive many other parameters. The refractive index $n(0)$ of studied alloys lie within $4 \leq x \leq 5.12$ and are shown in Fig. 6(a). The value of $n(\omega)$ is energy dependent which become maximum in around 1.5 eV and first minimum at 3 eV. Fig. 6(a) shows the plot of extinction coefficient $k(\omega)$ versus energy. The maxima of $k(\omega)$ is associated with zero of $\epsilon_{\text{real}}(\omega)$.

The other optical parameters like reflectivity (R), absorption coefficient $\alpha(\omega)$ and optical conductivity $\sigma(\omega)$ are also plotted in Fig. 6. The computed values of all these parameters are summarized in Table 4.

4. Conclusions

The structural, electronic and optical properties of $\text{YAuPb}_{1-x}\text{Six}$ ternary alloys were calculated using first principles approach. The effect of doping concentrations on the lattice parameter, bulk modulus, band gap energy, refractive index and dielectric constant was studied. A significant deviation from Vegard's law was observed in lattice parameter and bulk modulus calculation. The results of mechanical analysis revealed that these compounds have less compressibility and possess high elastic stability against deforming force. The calculated values of Pugh's ratio, Cauchy pressure and Poisson's ratio confirmed the brittle nature of these ternary alloys. Electronic properties calculated using mBj WC-GGA functional of DFT found more close to experimental results. All these compositions revealed a direct band gap structure except YAuSi . Complex dielectric analysis in terms of critical point structure gives symmetrical optical transition in these ternary alloys.

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