First-principles Computations of $Y_xGa_{1-x}As$ ternary alloys: A study on structural, electronic, optical and elastic properties

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ABSTRACT

In this work, first principles computational study on the structural, elastic, electronic and optical properties of Y$_x$Ga$_{1-x}$As as a function of yttrium concentration (x) are presented. The computations are performed within the full-potential (FP) linearized (L) augmented plane wave plus local orbital method designed within density functional theory (DFT). Firstly, we performed our calculations on the most stable phases, NaCl and Zincblende, then their transition pressure for each concentration is determined and analyzed. Our computed results for the zero yttrium concentration are found consistent with the available experimental measurements as well as with the theoretical predictions. Moreover, the dependencies of these parameters upon yttrium concentration (x) were found to be non-linear. We also report computed results on the electronic band structure, electronic energy band gap results, and density of states. A systematic study on the optical properties to analyze its optoelectronic character and elastic properties is presented.

Keywords: FP-LAPW; Y$_x$Ga$_{1-x}$As; Phase transition; Electronic properties; Optical constants


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1 Introduction

Semiconductor technology has made tremendous progress in recent years [1]. The trends of deriving the functionality of the materials have been widely extended by using the elements of the periodic table, to form new binary compounds as well as other innovative alloys. Gallium arsenide, GaAs belongs to III-V semiconductors and is considered an important material due to its versatile technological usage and flexibility of their physical properties via structural engineering. The functionality of novel properties could play an important role in optoelectronic and microelectronic components [2-9]. GaAs crystallizes in ZnS structure. The most important applications of GaAs are in photovoltaics, photodiodes, and optoelectronics such as Electro-Luminescent Diodes (LED) or Laser Diode (DL) [10-16]. Yttrium is a transition metal element and classified historically among the rare earth elements. Yttrium is a very soft metal which can be crushed into powder or compressed to chips very easily and may ignite vigorously if the temperature exceeds 400 °C. Furthermore, Yttrium is used in manufacturing LEDs or television cathode ray tubes, electrolytes, production of electrodes, lasers, electronic filters, superconductors, and in a variety of medical applications as well. Therefore, it creates high motivation to study the materials containing Y and other elements belonging to column eg., YAs [17-26]. The YAs crystallizes in NaCl structure, while, the arsenic atoms constitute a centered-face cubic lattice and Yttrium atoms occupy the middle of edges with an atom in the center of the cube with space group Fm3m (Oh) [27].

In this work, we focused our study on the YxGa1-xAs ternary alloys and their parent compounds GaAs and YAs. We searched for the most stable phases i.e. NaCl and Zinc blende structures and then determined the transition pressures by calculating the enthalpy at high pressures. Besides these, we have also studied the electronic, elastic and optical properties. Our paper is divided as follows: The second part discusses the computational method. The third part contains details of our results, interpretations, and comparison with the available
experimental measurements and computational predictions. Finally, in the last, conclusions are summarized.

2 Method of calculations

To do our computations, full-potential (FP) linearized (L) augmented plane wave (APW) plus local orbital (lo) abbreviated as FP-L(APW)+lo method framed within DFT [28] and realized in the computational code WIEN2k [29] was used to calculate the physical properties of ternary alloy, Y\textsubscript{x}Ga\textsubscript{1-x}As, at different concentration (x = 0, 0.25, 0.5, 0.75, 1). To incorporate exchange-correlation potential energy functional, an approximation (WC-GGA) called generalized gradient approximation (GGA) developed by Wu-Cohen was used [30]. Whereas, to deal with electronic properties GGA approximated by Engel-Vosko (EV-GGA) was applied as it is known to give better results for electronic properties [31]. To improve further the underestimated band gap results we have also used, Trans-Blaha modified Becke-Johnson (mBJ) exchange potential with the combination GGA correlation part- a semilocal exchange-correlation potential functional, mBJ-GGA, suggested by Trans-Blaha (TB-mBJ/GGA) [32].

To carry on computations in this method, FP-L(APW)+lo, the simulated unit/supercell is partitioned into two parts: the first part is considered around atoms in the form of muffin tin spheres (non-overlapping). In this region, the basis set was illustrated through a linear combination of the radial functions times of the spherical harmonics and maximum value \( l_{\text{max}} = 10 \) was used to expand the wave function in this region. Whereas in the second (interstitial) region, expansion of the basis set is done using plane waves and \( R_{\text{MT}}K_{\text{max}} = 8 \) was used to cut off the plane wave expansion (\( R_{\text{MT}} \) represents the smallest muffin tin radii and \( K_{\text{max}} \) for a maximum value of wave vector \( K \)). For Fourier expansion of the charge density, \( G_{\text{max}} = 14 \) was used. The Y (4d\textsuperscript{1}5s\textsuperscript{2}), Ga (3d\textsuperscript{10}4s\textsuperscript{2}4p\textsuperscript{1}) and As (3d\textsuperscript{10}4s\textsuperscript{2}4p\textsuperscript{3}) electrons are treated as valence electrons. The \( R_{\text{MT}} \) values for the atoms, Y, Ga and As were selected 2.5, 2.16 and 2.5a.u respectively. Special 32 k-points in the irreducible wedge for alloys and 47 for their binary...
counterparts were considered to perform integration in the reciprocal space over Brillouin zone for our calculations. These values of special k-points and $R_{MTK_{\text{max}}}$ were ensured by ensuring total energy convergence of the crystal to a lesser amount of $10^{-4}$ Ryd.

3 Results and Discussion

3.1 Structural properties and phase transition

A supercell was constructed with 8 atoms in periodically repeated ordered structures along x, y, and z-axis with lattice P (1x1x1). In a GaAs supercell, Yttrium atoms were added at the Ga sites as impurities by replacing the host Ga atoms per unit cell and different compositions are considered as $x = 0.25$, 0.5 and 0.75. By minimizing the total energy values, the structures of the doped systems were optimized with respect to lattice parameters. Firstly, we calculated the optimized volume (equilibrium volume) of the NaCl and Zinc blende structures of $Y_xGa_{1-x}As$ as shown in Figure 1. We have noticed that the zinc-blende phase of GaAs, $Y_{0.25}Ga_{0.75}As$, $Y_{0.5}Ga_{0.5}As$, and $Y_{0.75}Ga_{0.25}As$ are the most stable in their ground state, whereas YAs adopted the most stable NaCl structure. Our calculated equilibrium results of the lattice constants ($a$), bulk moduli ($B$) and the values of the transition pressure, $P_t$ using WC-GGA approximation are shown in Table 1, along with earlier reported results. These results were obtained using Muranghan's equation of state by fitting the computed results of total energies at equilibrium [43]. From the Table, we note, our obtained results at the level of WC-GGA for different structures of GaAs and YAs compounds are in good agreement with previously reported results in the literature. The obtained results for the lattice parameters as well as bulk moduli with varying concentration of Yttrium concentration, as $Y_xGa_{1-x}As$ ternary alloys are illustrated in Figures 2 and 3, respectively. We note that as a function of concentration, the lattice constant values increase linearly by following Vegard's law [44] with minor upward bowing parameter value i.e. -0.701 Å. However, for bulk modulus results, we see a large divergence from linear concentration dependence (LCD) pattern as for this case downward
bowing parameters is found 15.60 GPa for Y<sub>x</sub>Ga<sub>1-x</sub>As ternary alloys. To analyze the structural stability, Gibb's Free energy (G) calculations for both structures, NaCl and ZB i.e. by

\[ G = E + PV - TS \]

were done. Since the calculations for the total energy are done at \( T = 0 \); the relation \( G \) is reduced to enthalpy as \( H = E + PV \) [45]. The obtained results for the phase transition pressures for Y<sub>x</sub>Ga<sub>1-x</sub>As in both (ZB) and (NaCl) structures are given in Table 1 along with other results reported previously. As a prototype, we choose to represent just the transition pressure of concentration \( x=0.25 \) in Figure 4. The calculated transition pressure values \( P_t \) in Table 1 are presented for all concentrations. To find the concentration at which phase transition occurs, we calculate \( \Delta E_0 \) (\( E_{0ZB} - E_{0NaCl} \)) for each composition for Y<sub>x</sub>Ga<sub>1-x</sub>As ternary alloys, this variation is represented in Figure 5. It is clear that the transition from the ZB structure to NaCl takes place at \( x = 0.89 \).

3.2 Electronic band-structure and density of states

In this section, we discuss the band structure of the ternary alloy, Y<sub>x</sub>Ga<sub>1-x</sub>As for above-mentioned concentrations. The obtained results for the electronic band gap energy for different concentrations of Yttrium together with previously reported theoretical and experimental data are presented in Table 2. The electronic structure calculation of YAs using the EV-GGA or mBJ shows its metallic behavior. The calculated electronic band structures of ternary alloy Y<sub>x</sub>Ga<sub>1-x</sub>As for different concentrations, \( x=0, 0.25, 0.5 \) and \( 0.75 \) from both EV-GGA and TB-mBJ/GGA approximations demonstrate its direct band gap nature at the \( \Gamma \)-point. It can also be seen that the value of the electronic band gap energy of the GaAs computed via mBJ-GGA agrees well to available experimental data. The variation in the energy band gap for Y<sub>x</sub>Ga<sub>1-x</sub>As alloys using EV-GGA and mBJ-GGA as a function of \( Y \) concentration is shown in Figure 6. The results show a nonlinear variation in the band gap energy with concentration. The results obtained for the bowing parameter by employing quadratic fit are -1.498 eV and -1.395, respectively for the EV-GGA and mBJ-GGA.
approach. In this part, we have also determined and analyzed the DOS for further understanding the electronic properties of Y$_x$Ga$_{1-x}$As alloys. Figure 7 displays the total and partial DOS for binary compounds GaAs and YAs. For GaAs: the valence band can be divided into three main regions. The first is located in the range between -17 eV ~ -14 eV and is mainly contributed from the hybridization of Ga-p and As-s. The second is from -13 eV to -7 eV that can be regarded as the hybridization of Ga-d and As-s. The third region is from -6 eV to 0 eV as dominated by Ga-d and As-p. The band at above the E$_F$ is a mixture of As-p and Ga-d states. We notice a sharp peak located at -15 eV and dominated predominately by Ga-p states. For the semi-metallic YAs, the valence band is in the range from -11.0 to 0 eV, it is composed of As-s, As-p, and Y-d states. Hence it can be said that Y-d states make the major contribution in all energy regions, for the semi-metallic YAs. For Y$_x$Ga$_{1-x}$As, the profiles of density of states for compositions x = 0, 0.25, 0.5, 0.75, are similar. The valence band (VB) can be divided into three regions: the lower part of VB is dominated by Ga-p and As-s states, the second is contributed by Ga-d and As-s, and the upper part is dominated by As-p and Ga-d states. Hence, the conduction band is dominated by the d-states of Y along with the minute contribution of Ga-d and As-p states, respectively.

### 3.3 Optical properties

In order to analyze the optical behavior of the ternary alloy, Y$_x$Ga$_{1-x}$As, different optical parameters for different concentrations of Yttrium, for example, dielectric function (real and imaginary parts), absorption coefficient, refractive indices, and energy loss function were computed. We used the complex dielectric function to study the optical comportment of Y$_x$Ga$_{1-x}$As [49] i.e.,

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i \varepsilon_2(\omega)$$

(1)
The real part \( \varepsilon_1 \) is related to the polarization, while the imaginary part \( \varepsilon_2 \) reflects the absorption of the material. Generally, the real and imaginary parts \( \varepsilon_1 \) and \( \varepsilon_2 \) are related to so-called Kramers–Kronig relations [50] as:

\[
\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_{0}^{\infty} \frac{\varepsilon_2(\omega')}{(\omega'^2 - \omega^2)} d\omega' 
\]

\[
\varepsilon_2(\omega) = -\frac{2\omega}{\pi} P \int_{0}^{\infty} \frac{\varepsilon_1(\omega') - 1}{(\omega'^2 - \omega^2)} d\omega' 
\]

where \( \omega \) is used for frequency of the incident photons, and \( P \) is the main part of the Cauchy integral. Once \( \varepsilon_1 \) and \( \varepsilon_2 \) are determined, all other optical parameters can be derived easily from \( \varepsilon_1 \) and \( \varepsilon_2 \), for example, absorption coefficient, \( \alpha(\omega) \), the refractive index \( n(\omega) \) [51].

The absorption coefficient \( \alpha(\omega) \), refractive index \( n(\omega) \) are determined by using relations as given in the followings:

\[
\alpha(\omega) = \sqrt{2\omega} \left[ \varepsilon_2^2(\omega) + \varepsilon_1^2(\omega) - \varepsilon_1(\omega) \right]^{\frac{1}{2}} 
\]

\[
n(\omega) = \left( \frac{\varepsilon_1(\omega)}{2} + \sqrt{\frac{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}{2}} \right)^{\frac{1}{2}} 
\]

Following relation is obtained for the refractive index at low frequency and \( x = 0 \):

\[
n(0) = \varepsilon(0)^{\frac{1}{2}} 
\]

The reflection coefficient \( R(\omega) \) characterizes the part of the energy that is reflected at the interface of material. It is given by

\[
R(\omega) = \left| \frac{\sqrt{\varepsilon(\omega) - 1}}{\sqrt{\varepsilon(\omega) + 1}} \right|^2 
\]

The L(\( \omega \)) optical parameter called as electron energy loss function, is an important parameter which describes the loss of energy when a fast-moving electron is traversing through a material, it is defined by:
\[ L(\omega) = \varepsilon_2(\omega) / \left[ \varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) \right] \] (8)

The computed results for the \( \varepsilon_1 \) and \( \varepsilon_2 \) of the \( \varepsilon \) versus energy obtained for different considered concentrations is illustrated in Figures 8 and 9, respectively. It is clearly seen, that the threshold energy, \( \varepsilon_2(\omega) \) explains transitions at 0.58, 0.74, 0.58 and 0.47 eV that have been taken place in the \( \Gamma v - \Gamma c \) directions in the surrounding area of point \( \Gamma \) for GaAs, \( Y_0.5Ga0.5As \), \( Y_0.75Ga0.25As \), and \( Y_{0.25}Ga_{0.75}As \), respectively.

The principal peaks of \( \varepsilon_2(\omega) \) are situated at 4.32 in 26.50 eV, 3.13 in 20.60 eV, 2.52 in 15.01 eV, 4.12 in 14.35 eV and 1.35 in 12.55 eV (see Fig. 8) of \( x=0, 0.25, 0.5, 0.75 \) and 1, respectively. These peaks are attributable to direct transitions to conduction band from the valence band.

The values of the \( \varepsilon_1(0) \) and the index of refraction \( n(0) \) for various concentrations of Yttrium are given in Table 3. Our results agree with available data reported earlier in literature. The variations of the refractive index as a function of energy at different concentrations of Yttrium are shown in Figure 10. These curves show a maximum at energies 2.27, 1.80, 1.25, 1.21 and 0.91 eV for GaAs, \( Y_{0.25}Ga_{0.75}As \), \( Y_{0.5}Ga_{0.5}As \), \( Y_{0.75}Ga_{0.25}As \), and \( YAs \), respectively. We also note that these spectra show the presence of resonance in the ultraviolet, which corresponds to interband transitions. The variation of reflectivity as a function of energy at various concentrations of Yttrium is shown in Figure 11. These curves indicate a maximum value 60% at 4.57eV for GaAs, 53% at 7.74 eV for \( Y_{0.25}Ga_{0.75}As \), 45% at 5.13 eV for \( Y_{0.5}Ga_{0.5}As \), 43% at 7.14 eV for \( Y_{0.75}Ga_{0.25}As \) and 61% at 8.05 eV for \( YAs \). These results show that \( Y_{x}Ga_{1-x}As \) is a good candidate for using it as a base material for ultraviolet rays detector. In Figure 12, the variation of the \( L(\omega) \) versus energy for the considered concentrations is plotted. In the energy range 0 to 12 eV, we noticed that these spectra show minimal values because \( \varepsilon_2 \) has very important energy values [56]. The main peaks are
located around 15.94, 15.34, 14.22, 13.76 and 16.07 eV (>12 eV), these values are related to plasma resonance [57].

3.4 Elastic properties:

The elastic behavior of a solid is related to the rigidity of the atomic bonds and expresses the mechanical stability of the respective material. In this research work, the elastic constants of the Y$_x$Ga$_{1-x}$As (x= 0.25, 0.5, 0.75) alloys and their binary compounds are calculated. The elastic constants $C_{ij}$ are macroscopic parameters which give an insight view about the elastic properties of a material. Our studied materials need three elastic parameters i.e. $C_{11}$, $C_{12}$ and $C_{44}$. To evaluate these parameters of the studied materials, numerical calculations were performed within FP-L(APW+lo), by calculating the tensor components of $\varepsilon$ by employing deformations according to the Charpin method [58] and introduced in the code WIEN2k.

For an isotropic crystal, the expression which was used for computing the bulk modulus is as follows:

$$B = \frac{1}{3}(C_{11} + 2C_{12})$$  \hspace{1cm} (9)

Similarly Shear modulus, $G$ is described by following relation:

$$G = \frac{G_V + G_R}{2}$$  \hspace{1cm} (10)

Where $G_V = \frac{(2C + 3C_{44})}{5}$  \hspace{1cm} (11)

$$G_R = \left(\frac{6}{C} + \frac{9}{C_{44}}\right)^{-1}$$  \hspace{1cm} (12)

and $C = \frac{(C_{11} - C_{12})}{2}$  \hspace{1cm} (13)

$G_V$ and $G_R$ are Voigt shear modulus and Reuss shear modulus respectively. The anisotropy of the single crystal is defined by the Zener factor [59]:
\[ A = \frac{2C_{44}}{(C_{11} - C_{12})} \]  

(14)

However, Poisson’s ratio \( \nu \), shear constant \( C_s \), Kleinmann parameter \( \zeta \) and Young’s modulus \( Y \), are obtained by using relations [60–64]:

\[ \nu = \frac{3B - 2G}{6B + 2G} \]  

(15)

\[ Y = 9BG(3B + G) \]  

(16)

\[ C_s = \frac{1}{2}(C_{11} - C_{12}) \]  

(17)

\[ \zeta = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}} \]  

(18)

The values of \( C_{11}, C_{12} \) and \( C_{44} \), Shear modulus \( G \), bulk modulus \( B \), anisotropy parameter \( A \), ratio, \( B/G \), Young’s modulus \( Y \), Poisson ratio \( \nu \), Shear wave modulus \( C_s \) and Kleinman parameter \( \zeta \) for binary and ternary alloys of \( Y_xGa_{1-x}As \) are shown for concentrations (\( x = 0.25, 0.5, 0.75 \)) in Tables 4 and 5 along with available data reported earlier in literature. Our obtained results of elastic constants, satisfy mechanical stability conditions [71] i.e \( (C_{11} - C_{12}) > 0, C_{11} > 0, C_{44} > 0, (C_{11} + 2C_{12}) > 0 \). Similarly, our obtained bulk moduli \( B \) results also satisfy \( C_{12} < B < C_{11} \) criterion.

Moreover, we also noticed that the results of the bulk modulus obtained from the approach of total energy minimization as well as from the elastic constants were nearly the same.

According to Tables 4 and 5, we have found that the values obtained for the compound GaAs are in a nice agreement to the available theoretical predictions and experimental measurements. But for the YAs binary, until now we have not found experimental values, therefore we have just compared our results with the available theoretical predictions, and found that our results for YAs are also in good agreement as well. To our knowledge, there is
no data available in the literature concerning the theoretical and experimental results for our ternary alloys \((x = 0.25, 0.5, 0.75)\); so our results can be used as a reference.

From Table 4, the critical value of the \(B/G\) ratio obtained for our alloys is less than 1.70 \((B / G < 1.70)\). Thus, we can conclude that our alloys \(Y_xGa_{1-x}As\) are brittle materials. A material is said isotropic if \(A \approx 1\), while it is anisotropic if \(A \neq 1\). The \(Y_xGa_{1-x}As\) alloys have \(A \neq 1\) values, showing that our studied alloys are well anisotropic (see Table 5). It is observed that our calculated values of the Poisson’s ratio \(\nu\) are between -1 and 0.5 for \(Y_xGa_{1-x}As\). The calculated results of Young’s modulus highlights the stiffness of the material, i.e. material that has a larger value of \(Y\) is a more rigid material [72]. According to Table 5, the rigidity of our studied alloys has the following sequence: \(YAs > GaAs > Y_{0.75}Ga_{0.25}As > Y_{0.25}Ga_{0.75}As > Y_{0.5}Ga_{0.5}As\). From the \(C_S\) values, thus we found that the lattice stability of our studied alloys has the following sequence: \(YAs > GaAs > Y_{0.25}Ga_{0.75}As > Y_{0.5}Ga_{0.5}As > Y_{0.75}Ga_{0.25}As\).

It’s well known that the comparative locations for anions are indicated by Kleinman parameter \(\zeta\) and cations of the lattice when the crystal lattice is subjected to constant volume stress. The values of \(\zeta\) calculated for our material \(Y_xGa_{1-x}As\) \((x = 0.25, 0.5, 0.75)\) alloys and their binary compounds, implies that \(YAs\) is more resistant to variations in bond lengths or bond angles distortions than \(GaAs\), \(Y_{0.25}Ga_{0.75}As\), \(Y_{0.5}Ga_{0.5}As\), and \(Y_{0.75}Ga_{0.25}As\).

4 Conclusions

In this study, a first-principles computational study was carried out to determine structural, elastic, optical and thermal properties of the ternary alloy, \(Y_xGa_{1-x}As\) at different concentrations i.e. 0, 0.25, 0.5, 0.75 and 1.0. These computations were performed at the level of FP-L(APW)+lo structured within DFT. Our obtained results are summarized as follows;

- Our computed results of the lattice parameters, bulk moduli, and transition pressure were found in nice agreement with the available experimental and theoretical data.
- The obtained results showed the ZB structure most stable one and found its transition at concentration, \( x = 0.89 \).

- The lattice parameter value was found to be varied linearly with the doping concentration of Y impurities, following the Vegard law. However, for bulk modulus, a deviation from LCD has been observed.

- The computed results of the electronic band structure confirmed direct band gap of the \( \text{Y}_x\text{Ga}_{1-x}\text{As} \) ternary alloy. The varying values of the band gap energy with respect to concentration showed a non-linear trend. This deviation indicates the disorder in the alloy (shows bowing parameter). Binary YAs was found metal in nature but GaAs and YGaAs alloys were found in semiconductor nature.

- The optical properties as a function of concentrations were also predicted.

- The study of the elastic properties allowed us to conclude that the studied alloys were showed a slight elastic anisotropy in shear. In addition, the values of the elastic constants indicated the mechanical stability of the \( \text{Y}_x\text{Ga}_{1-x}\text{As} \) alloy in the studied structure i.e. the \( B / G \) values showed these alloys fragile materials.

- Our computed results were found in good agreement with experimental measurements and theoretical predictions wherever were available. But unfortunately for the concentrations (\( x = 0.25, 0.5, 0.75 \)) there are no experimental results to make a comparison.

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**Figure captions**

**Figure 1:** Variation of total energy versus volume for zinc blend and NaCl structures of $Y_xGa_{1-x}As$ for the considered concentrations.

**Figure 2:** Composition dependence of the calculated lattice constants for $Y_xGa_{1-x}As$ alloy.

**Figure 3:** Composition dependence of the calculated bulk modulus for $Y_xGa_{1-x}As$ alloy.

**Figure 4:** Calculated enthalpy as a function of pressure for $Y_{0.25}Ga_{0.75}As$ alloy.

**Figure 5:** The variation of the $\Delta E_0$ as a function of the composition for ternary alloys $Y_xGa_{1-x}As$.

**Figure 6:** Band gaps energies of the $Y_xGa_{1-x}As$ alloys as a function of Y concentrations using EV-GGA and mBJ schemes.

**Figure 7:** Calculated total density of states (DOS) of binary compounds GaAs and YAs.

**Figure 8:** Calculated imaginary part of dielectric function for $Y_xGa_{1-x}As$.

**Figure 9:** Calculated real part of the dielectric function for $Y_xGa_{1-x}As$.

**Figure 10:** Calculated refractive index for $Y_xGa_{1-x}As$.

**Figure 11:** Calculated reflectivity of $Y_xGa_{1-x}As$.

**Figure 12:** Calculated energy loss function $L(\omega)$ of $Y_xGa_{1-x}As$. 
Figure 1
Figure 2

Figure 3
Figure 4

- A graph showing the enthalpy (Ry) as a function of pressure (GPa) for different compositions of \( Y_xGa_{1-x}As \). The graph includes lines for ZB and NaCl structures, with a specific point marked at \( x=0.25 \) and \( P=5.05 \) GPa.

Figure 5

- A graph showing the difference in energy \( E_{ZB} - E_{NaCl} \) (eV) as a function of composition \( X \). The graph includes data points and a dashed line indicative of the trend.
Figure 6
Figure 7
Figure 8

Figure 9
Figure 12
Table captions

**Table 1:** Calculated lattice constant $a$ (in Å), bulk modulus $B$ (in GPa) and values of the transition pressure $P_t$, for $Y_xGa_{1-x}As$ alloys and their binary compounds, compared to the experimental and other theoretical works.

<table>
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<th>$x$</th>
<th>This work</th>
<th>Exp</th>
<th>Other works</th>
<th>This work</th>
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<th>This work</th>
<th>Exp</th>
<th>Other works</th>
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<td>5.65$^{a,b}$</td>
<td>5.610$^c$</td>
<td>69.520</td>
<td>76$^d$, 77$^h$</td>
<td>75.81$^c$</td>
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<td>16.6$^j$</td>
<td>10.5$^e$</td>
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<td>8.015$^d$</td>
<td>83.166</td>
<td>77$^i$, 76.80$^d$</td>
<td>57.35</td>
<td>58.25$^j$, 50.45$^f$, 56$^k$</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$^a$ Ref. [33], $^b$ Ref. [34], $^c$ Ref. [35], $^d$ Ref. [36], $^e$ Ref. [37], $^f$ Ref. [18], $^g$ Ref. [38], $^h$ Ref. [39], $^i$ Ref. [40], $^j$ Ref. [24], $^k$ Ref. [41], $^l$ Ref. [42]

**Table 2:** Band gap energies $E_g$ (eV) for $Y_xGa_{1-x}As$ alloys at various compositions.

<table>
<thead>
<tr>
<th>$x$</th>
<th>This work</th>
<th>Exp</th>
<th>Other calculations</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EV-GGA</td>
<td>mBJ</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>1.004</td>
<td>1.595</td>
<td>1.424$^c$</td>
</tr>
<tr>
<td>0.25</td>
<td>0.96</td>
<td>1.397</td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>0.737</td>
<td>0.87</td>
<td></td>
</tr>
<tr>
<td>0.75</td>
<td>0.421</td>
<td>0.600</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>-0.232</td>
<td>-0.337</td>
<td>-0.356$^b$</td>
</tr>
</tbody>
</table>

$^a$ Ref. [46], $^b$ Ref. [47], $^c$ Ref. [48].
### Table 3: Optical dielectric constants $\varepsilon_1 (0)$ and index of refraction n(0) of $\text{Y}_x\text{Ga}_{1-x}\text{As}$ for different compositions x.

<table>
<thead>
<tr>
<th>x</th>
<th>$\varepsilon_1 (0)$</th>
<th>n(0)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>This work</td>
<td>Exp</td>
</tr>
<tr>
<td>0</td>
<td>13.92</td>
<td>13.20$^a$</td>
</tr>
<tr>
<td>0.25</td>
<td>13.54</td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>13.28</td>
<td></td>
</tr>
<tr>
<td>0.75</td>
<td>11.27</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>19.96</td>
<td></td>
</tr>
</tbody>
</table>

$^a$ Ref. [52], $^b$ Ref [53], $^c$ Ref [54], $^d$ Ref. [55], $^e$ Ref. [35].

### Table 4: Calculated values of elastic constants $C_{11}$, $C_{12}$ and $C_{44}$ (in GPa), bulk modulus B (in GPa), shear modulus G (in GPa), ratio B/G, for $\text{Y}_x\text{Ga}_{1-x}\text{As}$ (x= 0.25, 0.5, 0.75) alloys and their binary compounds, compared to the experimental and other theoretical works :

<table>
<thead>
<tr>
<th></th>
<th>$C_{11}$ (GPa)</th>
<th>$C_{12}$ (GPa)</th>
<th>$C_{44}$ (GPa)</th>
<th>B (GPa)</th>
<th>G (GPa)</th>
<th>B/G</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>GaAs</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Our work</td>
<td>100.075</td>
<td>59.363</td>
<td>83.267</td>
<td>72.933</td>
<td>47.669</td>
<td>1.52</td>
</tr>
<tr>
<td>Exp</td>
<td>106.5$^a$</td>
<td>53.3$^a$</td>
<td>60.2$^a$</td>
<td>75.5$^a$</td>
<td>32.6$^a$</td>
<td></td>
</tr>
<tr>
<td>Other works</td>
<td>106.5$^b$, 122.3-147.6$^c$</td>
<td>60.2$^b$, 40.6-119$^d$</td>
<td>33.6$^b$, 42.4-107$^c$</td>
<td>75.6$^b$, 70.8-135$^c$</td>
<td>75.6$^b$, 70.8-135$^c$</td>
<td></td>
</tr>
<tr>
<td><strong>Y_{0.25}Ga_{0.75}As</strong></td>
<td>80.326</td>
<td>46.992</td>
<td>58.778</td>
<td>58.104</td>
<td>35.583</td>
<td>1.632</td>
</tr>
<tr>
<td>Our work</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Y_{0.5}Ga_{0.5}As</strong></td>
<td>69.349</td>
<td>44.770</td>
<td>59.03</td>
<td>52.963</td>
<td>31.872</td>
<td>1.661</td>
</tr>
<tr>
<td>Our work</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Y_{0.75}Ga_{0.25}As</strong></td>
<td>56.380</td>
<td>51.106</td>
<td>26.504</td>
<td>52.864</td>
<td>44.802</td>
<td>1.179</td>
</tr>
<tr>
<td>Our work</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>YAs</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Our work</td>
<td>202.382</td>
<td>23.869</td>
<td>43.871</td>
<td>83.373</td>
<td>58.548</td>
<td>1.423</td>
</tr>
<tr>
<td>Exp</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Other works</td>
<td>192$^d$, 183$^e$, 156$^f$</td>
<td>33$^d$, 39$^e$, 41$^f$</td>
<td>19$^d$, 23$^e$, 41$^f$</td>
<td>86$^d$, 76$^e$, 79$^f$</td>
<td>45$^d$, 35$^f$</td>
<td></td>
</tr>
</tbody>
</table>

$^a$ Ref. [65], $^b$ Ref. [66], $^c$ Ref. [67], $^d$ Ref. [68], $^e$ Ref. [24], $^f$ Ref. [41].
Table 5: calculated values of Anisotropy parameter $A$, Poisson ratio $\nu$, Young’s modulus $Y$ (in GPa) shear wave modulus $C_s$ (in GPa) and Kleinman parameter $\zeta$ for $Y_xGa_{1-x}As$ ($x=0.25, 0.5, 0.75$) alloys and their binary compounds, compared to the experimental and other theoretical works

<table>
<thead>
<tr>
<th></th>
<th>$A$</th>
<th>$\nu$</th>
<th>$Y$ (GPa)</th>
<th>$C_s$ (GPa)</th>
<th>$\zeta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$GaAs$</td>
<td>4.09</td>
<td>0.231</td>
<td>117.424</td>
<td>20.356</td>
<td>0.701</td>
</tr>
<tr>
<td>Our work</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exp</td>
<td></td>
<td>0.31$^a$</td>
<td>85.5$^b$</td>
<td>-</td>
<td>0.58$^c$</td>
</tr>
<tr>
<td>Other works</td>
<td></td>
<td>0.36$^d$</td>
<td>63.0$^d$</td>
<td>-</td>
<td>0.67$^d$, 0.81$^e$</td>
</tr>
<tr>
<td>$Y_{0.25}Ga_{0.75}As$</td>
<td>3.526</td>
<td>0.245</td>
<td>88.653</td>
<td>16.667</td>
<td>0.695</td>
</tr>
<tr>
<td>Our work</td>
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<tr>
<td>$Y_{0.5}Ga_{0.5}As$</td>
<td>4.803</td>
<td>0.249</td>
<td>79.640</td>
<td>4.800</td>
<td>0.743</td>
</tr>
<tr>
<td>Our work</td>
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<tr>
<td>$Y_{0.75}Ga_{0.25}As$</td>
<td>10.05</td>
<td>0.169</td>
<td>104.800</td>
<td>2.637</td>
<td>0.936</td>
</tr>
<tr>
<td>Our work</td>
<td></td>
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</tr>
<tr>
<td>$YAs$</td>
<td>0.491</td>
<td>0.215</td>
<td>142.329</td>
<td>89.256</td>
<td>0.268</td>
</tr>
<tr>
<td>Our work</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exp</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Other works</td>
<td>0.33$^f$, 0.67$^g$, 0.48$^h$</td>
<td>0.22$^f$, 0.21$^f$</td>
<td>111$^i$, 104$^i$</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

$^a$ Ref. [69], $^b$ Ref. [65], $^c$ Ref. [70], $^d$ Ref. [66], $^e$ Ref. [67], $^f$ Ref. [68], $^g$ Ref. [41], $^h$ Ref. [24].