Properties of group III–V semiconductor: BAs

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Abstract. The structural, electronic, mechanical, thermal and optical properties of boron arsenide (BAs) semiconductor, which belongs to group III–V, has been studied using the first-principles approach. BAs is a binary semiconductor compound, which has a space group $F-43m$ at ambient temperature. The structural and electronic properties of BAs are found to be in good agreement with the available experimental and theoretical results. Some of the mechanical properties are also in agreement with the data available. The thermal parameters such as Debye temperature, specific heat and Grüneisen parameter are analysed as functions of temperature and pressure.

Keywords. Semiconductors; *ab-initio* PBEsol-GGA; computational studies; mechanical and physical properties; density functional theory.

1. Introduction

Among group III–V semiconductors, boron compounds have attracted great attention, in recent years, due to various technological applications. These compounds have applications in electronic devices, optical devices that operate in the short wavelength range of the visible spectrum and in devices operating at high temperatures. The boron arsenide (BAs) compound has unique physical properties [1]. It possesses low density, low dielectric constant [2] and extremely high thermal conductivity [3,4]. It also possesses an important characteristic related to inverse contribution between anions and cations. There are some studies, which show that boron's contribution in BAs is that of an anion which is due to its small size and absence of p-electrons from the core of the B atom [5]. In an experimental work [6], BAs was reported as an acceptable candidate for photovoltaic and photo-electrochemical applications. *Ab initio* calculations using plane-wave expansion within the local density approximation (LDA) and pseudo-potential approximation have been used to calculate the electronic properties of BX (X = N, As and Sb) compounds [7].

Total energy calculations for structural and elastic properties of the boron compounds, such as BP, BAs and BSb have been carried out using augmented plane wave + local orbital method with the local density approximation and generalized gradient approximation [8]. BAs is gaining interest, both experimentally as well as theoretically, because of its potential characteristic advantages [7–9]. The experimental value of bulk modulus of BAs has been reported as 148 GPa [10] and its lattice constant in zinc blende structure at room temperature has been reported as 4.777 Å [11]. A self-consistent orthogonalized-plane wave has been used for energy-band calculation using a non-relativistic formalism and Slater's

free electron exchange approximation. In the same paper, imaginary part of the dielectric constant, spin orbit splitting, effective masses, deformation energies and the form factors have also been calculated [12].

Experimental band gap of zb-BAs has been reported as 1.46 eV [6,13]. The effect of vacancies on lattice thermal conductivity has been reported theoretically for BAs [14].

In 2008, Perdew, Burke and Ernzerhof (PBE) revised the generalized gradient approximation known as PBE-GGA [15] and introduced a new gradient level functional known as PBEsol-GGA [16]. The authors removed the traditional predictions, which were related with the atomic energies by restoring the first-principles gradient expansion for the exchange and re-adjusting the correlation term using the jellium surface exchange–correlation energies obtained at the meta-GGA level [17]. The new GGA functional, referred as PBEsol-GGA has been designed to yield improved equilibrium properties of densely packed solids and most importantly, to remedy the deficiencies of the GGA functional for the surface [18–20].

In spite of the above-mentioned information about BAs, still the degrees of anisotropy, linear compressibility, compliance constant, sound velocity, thermal properties and optical conductivity have not been reported in the literature. Also, for many parameters, the result reported by different researchers are not in agreement with each other as they have used different approaches.

The aim of this paper is to provide a comparative and supportive study on the physical properties like structural, electronic, optical, mechanical and thermal properties of BAs using PBEsol-GGA functional employing the full-potential augmented plane-wave method within the framework of the density functional theory (DFT).

2. Computational details

Self-consistent calculations of total energies of BAs based on full potential ‘linearized augmented plane wave’ method is carried out using the WIEN2K code [21]. In the unit cell of zinc blende structure of BAs, the atomic positions of B and As are taken at (0, 0, 0) and (1/4, 1/4, 1/4) and their muffin tin radius taken as 1.6 and 2.0 Bohr, respectively. The unit cell is divided into non-overlapping spheres around atoms and the interstitial region. The wave functions inside the muffin-tin spheres are expanded in terms of spherical harmonics, while for interstitial region, the plane-wave expansions have been used.

To obtain the total energy convergence, we have expanded the Kohn–Sham wave functions up to $R_{MT} \times K_{max} = 7$ (R_{MT} is the plane wave radii and K_{max} is the maximum reciprocal lattice vector). Partial waves used inside atomic spheres have been expanded up to $l_{max} = 10$. In charge density Fourier expansion magnitude of the largest vector is taken as $G_{max} = 12$. The cut-off energy for separating core from valence states is set to -6 Ry. The convergence criterion for energy and charge have been taken as 10^{-4} Ry and 10^{-3} e $^{-}$, respectively.

3. Calculations, results and discussion

3.1 Structural properties

The structural parameters are obtained by the process of optimization of the unit cell volume corresponding to the total energy of BAs. Minimization of the total energy (shown in figure 1) depending on the unit cell volume of BAs has been obtained by fitting a set of the unit cell volume and corresponding conversed value of the total energy of BAs to the Murnaghan equation of state [22]:

$$E(V) = E_0 + \frac{B_0 V}{B'_0} \left[\frac{(V_0/V)^{B'_0}}{B'_0 - 1} \right] - \frac{B_0 V_0}{B'_0 - 1}. \quad (1)$$

Here, E_0 is the equilibrium energy, B_0 the bulk modulus and B'_0 the first pressure derivative of B_0 .

The structural optimization results obtained for BAs are shown in table 1 along with the earlier reported experimental as well as the theoretical results. From the table, it is clear that our obtained lattice constant is in good agreement with the experimental results in comparison to the other results except that obtained using PWPP-LDA in [24].

3.2 Electronic properties

3.2a Energy bands and DOS: Energy bands of zb-BAs along with total and partial density of states (DOS) obtained using the PBEsol-GGA approximation are shown in figure 2a and b. Figure 2a shows the electronic band structure and the total DOS. According to our calculation, the obtained value of Γ –X indirect band gap is 1.20 eV. It is less than the reported

Table 1. Calculated lattice constants (a in Å), bulk modulus (B in GPa), bulk modulus pressure gradient B' and energy band gap (E_g in eV) for BAs in zinc blende phase along with earlier reported experimental and theoretical results.

Method	A	B	B'	E_g	Ref.
PBEsol-GGA	4.770	140	4.16	1.20	Present work
Experimental	4.777	—	—	—	[23]
Experimental	—	—	—	1.46	[6,13]
LDA	4.743	152	3.65	1.12	[8]
GGA	4.812	133	3.75	1.21	[8]
PWPP-LDA	4.777	145	—	1.25	[24]
PWPP-LDA	4.728	141	4.00	1.06	[7,9]
FP-LAPW-GGA	4.784	137	3.49	1.23	[25]
FP-LAPW-GGA	4.812	131	3.71	—	[26]
LDA	4.733	146	4.18	—	[27]
PBE-GGA	4.810	131	3.93	—	[27]
PW-GGA	4.806	131	3.43	—	[27]
EV-GGA	5.061	86	3.88	—	[27]
FP-LDA	4.741	147	4.22	—	[28]
FP-GGA	4.817	131	4.17	—	[28]

Figure 1. Total energy vs. volume using the PBE-sol approximation for BAs binary compound.

experimental value of the energy band gap, 1.46 ± 0.02 eV [6]. On the other hand, direct band gap at Γ – Γ is found as 3.16 eV and that of Γ –K and Γ –W are obtained as 1.80 and 5.07 eV, respectively. In tabular form it is listed as follows:

Valence band maxima	Conduction band minima	Type of gap	Gap (eV)
Γ	X	Indirect	1.20
Γ	Γ	Direct	3.16
Γ	K	Indirect	1.80
Γ	W	Indirect	5.07
		Experimental	1.46 ± 0.02

In figure 2a, the most prominent DOS peaks in the valence band region lie at -11.37 , -8.03 and -3.97 eV. The conduction band region’s first dense and sharp peak

Figure 2. (a) Band structure of BAs along with DOS plot. (b) Partial DOS of BAs. Vertical line corresponds to the position of the Fermi energy level. (c) Energy band gaps as a function of lattice parameter a . Vertical broken line corresponds to the equilibrium lattice constant.

is shown at 3.50 eV and the second peak is seen at 4.75 eV.

Contributions of the s-, p- and d-orbitals in total DOS are shown in the form of partial DOS. The lowest valence band region is dominated by 3s states of arsenide and also insignificant contribution of 2s orbital of boron. The upper part of the valence band is mostly dominated by 3p states of As and 2s and 2p states of boron. In the conduction band, there is a significant contribution of 2s and 2p states of B, along with the contributions of 3s, 3d and 3p states of As.

Energy gaps between the top of the valence band and the bottom of the conduction band as a function of the lattice parameters in BAs are plotted in figure 2c. The indirect band gap Γ -L and direct band gap Γ - Γ decreases with the increase in lattice parameter, while indirect band gaps Γ -X, Γ -K show a very small increment with increase in the value of lattice parameter. Band gaps Γ -W show no effect of the lattice parameter.

3.2b Electronic charge density: Figure 3a and b shows the characteristic bonding and charge density between atoms. The analysis shows that the highest density of charge is distributed in the immediate vicinity of the atomic sites, but it is not distributed spherically symmetric. This shows covalent nature of bonding in BAs. The size of humps in figure 3b reveals that arsenic is more electronegative than boron.

3.3 Elastic properties

Hardness of the cubic material is defined by constants C_{11} , C_{12} and C_{44} , known as elastic stiffness constants [29]. Value of these constants is obtained from total energy calculations and is used to represent the single crystal elastic properties. The relationship between dynamical behaviour and the mechanical properties of the crystal is established by the elastic constants, which gives information about the nature of the forces acting on a solid. These constants also give information about stiffness and elastic stability of the material. C_{11} indicates the longitudinal elastic behaviour of the material, and C_{12} and C_{44} indicate the off diagonal and the shear elastic characteristics of the cubic crystal. It has been observed that C_{11} is more sensitive to pressure than C_{12} and C_{44} , because longitudinal strain produces change in volume without changing its shape and this change in volume is related to the applied pressure. On the other hand, a shearing or transverse strain produces a change in shape without changing its volume [29]. To attain the mechanical stability, the cubic crystals should satisfy the following stability conditions [30]:

$C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$ and $C_{12} < B < C_{11}$.

In the above stability conditions, B refers to the bulk modulus. It defines the strength of bonds in solids and is a measure of resistance to external deformation. It is also known as the reciprocal of compressibility, β [8,31,32]:

$$B = \frac{1}{\beta} = \frac{C_{11} + 2C_{12}}{3}. \quad (2)$$

When a shearing force is applied on the material, resistance offered by the material to the change in shape is defined as shear modulus or modulus of rigidity [33,34]. It is denoted by C_S and is given by the relation [35]:

$$C_S = \frac{C_{11} - C_{12}}{2}, \quad (3)$$

$$G = \frac{G_V + G_R}{2}, \quad (4)$$

G is the isotropic shear modulus, where G_V is Voigt's shear modulus corresponding to upper bound G values, and G_R is the Reuss's shear modulus corresponding to the lower bound G values, and can be written as [26]

$$G_V = \frac{C_{11} - C_{12} + C_{44}}{5}, \quad \text{and} \quad \frac{5}{G_R} = \frac{4}{C_{11} - C_{12}} + \frac{3}{C_{44}}. \quad (5)$$

When tension is applied along a single axis, the resistance offered by the material gives the degree of stiffness of the material. It is denoted by Y and is known as Young's modulus. Relationship among Y , G and B is given as [26,36,37]:

$$Y = \frac{9GB}{G + 3B}. \quad (6)$$

Brittleness and ductility are very important characteristics of materials. Materials, which are brittle in nature, deform less or do not even deform when subjected to stress before the material breaks. On the other hand, materials that are ductile in nature deform a lot before fracture. The point that defines the limit of ductility or brittleness of the material is defined as Pugh ratio [38,39]. It is given as follows:

$$\text{Pugh ratio} = \frac{G}{B}. \quad (7)$$

If the value of Pugh ratio is equal to or > 1.75 , the material shows a ductile nature, otherwise it shows brittle nature. For BAs, obtained value of the Pugh ratio is 0.9647 which is < 1.75 , therefore it is brittle in nature.

Cauchy pressure (C_P) also defines the brittle or ductile nature of the material; its positive value shows the ductile nature, whereas the negative value defines the brittle nature [30,40]. It is calculated using the below equation:

$$C_P = C_{12} - C_{44}. \quad (8)$$

For BAs, the obtained value of C_P -99.273 GPa, and also supports brittle nature of BAs [39,40].

The Poisson ratio (ν) gives detailed information about the bonding force in materials and is defined as the ratio of transverse strain to longitudinal strain in elastic loading direction [41,42]. For solids, its lower and upper limits are, respectively, $\nu = 0.0$ and $\nu = 0.5$. Its value is obtained using the

Figure 3. (a) Contour plot and (b) total electronic charge distribution plots of BAs in the (0 1 1) plane.

below equation [26]:

$$\nu = \frac{1}{2} \left[\frac{3B - 2G}{3B + G} \right]. \quad (9)$$

Kleinman internal strain parameter (ζ) for cubic materials describes the relative ease of bond bending to the bond stretching. Minimizing bond bending leads to $\zeta = 0$ and minimizing bond stretching leads to $\zeta = 1$ [43]. It is derived using the below equation:

$$\zeta = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}}. \quad (10)$$

The obtained value of ζ for BAs is 0.409, which shows that there is a very slight internal displacement due to strain [39].

The elastic anisotropy or Zener anisotropy factor of crystals has an important implication in engineering, since it is correlated with the possibility to persuade microcracks in the materials [39], if the value of $A = 1$, then the material is isotropic in nature. If the value of A is greater than or smaller than 1, it gives the measure of the degree of elastic anisotropy [30,44]. Its value is obtained using the below equation:

$$A = \frac{2C_{44}}{(C_{11} - C_{12})}. \quad (11)$$

For BAs, $A = 1.675325$. It clearly indicates that BAs is anisotropic in nature [30].

Isotropy factor is inverse of Zener anisotropy factor, which is given by the following equation [45]:

$$A^{-1} = \frac{C_{11} - C_{12}}{2C_{44}}. \quad (12)$$

Degree of elastic anisotropy for cubic crystal can be calculated using the following equation [30]:

$$A^* = \frac{3(A - 1)^2}{3(A - 1)^2 + 25A}. \quad (13)$$

The Cauchy discrepancy parameter C^* , the Cauchy coefficient C_a and the Born ratio B_0 for the cubic crystal are related to the stiffness constants as follows [35]:

$$C^* = \frac{C_{12} - C_{44}}{C_{12} + C_{44}}, \quad (14)$$

$$C_a = \frac{C_{12}}{C_{44}}, \quad (15)$$

$$B_0 = \frac{(C_{11} + C_{12})^2}{4C_{44}(C_{11} - C_{44})}. \quad (16)$$

Linear compressibility [46] is expressed as

$$C_0 = \frac{1}{C_{11} + 2C_{12}}. \quad (17)$$

3.3a Compliance constant: Flexibility or compliance is defined as reciprocal of stiffness. Flexibility represents the tolerance of the semiconductor when it undergoes elastic deformation i.e., materials which can be easily deformed are known as flexible materials. These materials have low elastic modulus and a very small stress is sufficient to produce strain. Materials which are highly compliant can be easily deformed.

Relationships between stiffness constant C_{ij} and elastic compliance S_{ij} [46] are given as follows:

$$S_{11} = \frac{C_{11} + C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})}, \quad (18)$$

$$S_{12} = \frac{-C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})}, \quad (19)$$

Table 2. Various parameters related to the mechanical stability and nature of BAs compound in zinc blende phase.

Parameter	Present work	Earlier reported results												
		[39]	[35]	[47]	[26]	[48]	[8]	[8]	[49]	[50]	[51]	[52]	[53]	[48]
C_{11} (GPa)	275		289	410	267	289	295	275	279	291	291	218	274	279
C_{12} (GPa)	71		77	166	64	70	78	63	120	73	72	95	70	120
C_{44} (GPa)	170		129	51	162	160	177	150	113	158	157	112	123	113
$B(1/\beta)$ (GPa)	139													173
C_s (GPa)	102		106	122	101	109	108	106	79	109	109	61	102	79
G (GPa)	138.72				134									
Y (GPa)	312.43				300									
Pugh ratio	0.96	1.02												
C_p (GPa)	−99.27	−99												
ν	0.12	0.12			0.118									
ζ	0.41		0.52		0.39					0.4	0.36	0.57	0.41	
A	1.67				1.59									
A^{-1}	0.59													0.704
A^*	0.01													
C^*	−0.41		−0.25											
C_a	0.42		0.59							1.06				1.06
B_0	3.36		1.63							0.86				0.85
$C_0 \times 10^{-3}$ (GPa $^{-1}$)	2.30													1.93
$S_{11} \times 10^{-3}$ (GPa $^{-1}$)	4.07													4.84
$S_{12} \times 10^{-4}$ (GPa $^{-1}$)	−8.39													−14.5
$S_{44} \times 10^{-3}$ (GPa $^{-1}$)	5.86													8.85

Table 3. Calculated sound velocities in three different directions in zinc blende phase of BAs obtained using the values of the second-order elastic constants (in 10^5 cm s $^{-1}$).

Direction of propagation	Plane of polarization	Mode	Sound velocity (present work)	Theoretical [46]
[1 0 0]	[1 0 0]	LA	7.25	7.31
	(1 0 0)	TA ₁ , TA ₂	5.717	4.65
[1 1 0]	[1 1 0]	LA	8.11	7.73
	(1 1 0)	TA ₁	4.417	3.90
	(0 0 1)	TA ₂	5.717	4.65
[1 1 1]	[1 1 1]	LA	8.38	7.87
	(1 1 1)	TA ₁ , TA ₂	4.889	4.17

$$S_{14} = \frac{1}{C_{44}}. \quad (20)$$

For cubic lattice, the velocity of sound travelling in three major directions [1 0 0], [1 1 0] and [1 1 1] [46] plays an important role. Acoustic waves are the mechanical waves that cannot travel through a vacuum. These waves are known as elastic waves when they pass through a solid. These waves are different from the electromagnetic (EM) waves. When they pass through liquid or gas, they are known as acoustic waves.

The major difference between EM waves and acoustic waves is that EM waves are polarized in two independent directions, whereas in homogeneous solids, acoustic waves have three independent directions of polarization. Two along transverse directions known as shear waves and they

are denoted by TA₁ and TA₂ and other along longitudinal direction is known as compression wave denoted by LA. The velocity of sound has been calculated using the below equation [46]:

$$v = \sqrt{\frac{C_{ij}}{g}}, \quad (21)$$

where v is the sound velocity, C_{ij} is the second-order elastic stiffness constant and g is the crystal density.

Computed values of all the above mentioned parameters related to the mechanical stability of BAs along with the earlier reported results are summarized in table 2. The velocity of sound in all the three high symmetry directions i.e., [1 0 0], [1 1 0] and [1 1 1] in BAs is listed in table 3.

Figure 4. Calculation of various thermodynamical parameters as a function of temperature at different pressures: (a) primitive unit cell volume V , (b) bulk modulus B , (c) Debye temperature θ_D , (d) thermal expansion coefficient α , (e) specific heat capacity at constant volume C_V , (f) specific heat capacity at constant pressure C_P , (g) entropy S and (h) internal energy U .

3.4 Thermal properties

To investigate the thermodynamic properties of BAs under high temperature and high pressure, we apply the

quasi-harmonic Debye approximation as implemented in the Gibbs programme [54]. The study of thermal properties gives information about phase stability, melting point, strength and nature of bonding. The thermal properties are determined in

the temperature range from 0 to 1000 K and pressure range 0–50 GPa. The thermal properties of BAs are reported for the first time. Graphical representation of the thermal parameters is shown as a function of temperature for the different values of pressure.

Figure 4a shows variation in primitive unit cell volume as a function of temperature at different pressures. The graph interprets that volume gradually increases with temperature at constant pressure. On the other hand, as pressure increases at a given temperature, volume decreases.

In figure 4b, we observe that there is a small variation in bulk modulus up to 100 K, after which it decreases linearly with the increase in temperature. It is also observed that bulk modulus increases with increase in pressure.

The Debye temperature (θ_D) is an essential thermodynamical quantity used to describe various properties of materials that are related to lattice vibrations [55]. The Debye temperature is related to quantities, such as elastic constant, pressure, lattice thermal conductivity and specific heat [56]. Binding forces are related to hardness of the material, and higher the hardness of the material, the higher is the Debye temperature [57]. Figure 4c shows the variation of Debye temperature θ_D with temperature and pressure. In our results, we find that there is a minor variation in θ_D up to 0–100 K, but above 100 K, θ_D decreases linearly as temperature increases. The results also show that θ_D increases with the increase in pressure.

The thermal expansion coefficient α , is an important parameter which provides information about the anharmonic properties of the material. Figure 4d shows the variation of thermal expansion coefficient with temperature at different pressures. It is observed that α increases rapidly with increase in temperature, especially at zero pressure, and decreases with increase in pressure. Above 400 K, α increases linearly with temperature and becomes almost constant.

The heat capacity of a substance gives information about the vibrational properties of the material. Figure 4e shows variation in specific heat at constant volume at different pressures and different temperatures. It is observed that from 0 to 600 K, the value of specific heat capacity increases rapidly with increase in temperature and pressure. At high pressure, C_v is close to a constant value of $49.4 \text{ J mol}^{-1} \text{ K}^{-1}$, which is the so-called Duong–Petit limit [58], and this limit is common for all solids at high temperature. The results show that at zero pressure, C_v increases rapidly with temperature, but as pressure increases, this variation is not so rapid.

Figure 4f represents heat capacity at constant pressure (C_p) with temperature at various pressures. The graph obtained for C_p at low temperature is similar to that of C_v . Similar to C_v , C_p also decreases with the increase in pressure, but it does not converge to a constant value. At room temperature and zero pressure, the value of C_p is $48.7 \text{ J mol}^{-1} \text{ K}^{-1}$.

The entropy is defined as a measure of disorder in a crystal. Figure 4g shows the variation of entropy S with pressure and temperature. As temperature increases, the vibration of atoms increases inside, i.e., entropy increases. It is

important to know that as temperature increases, contribution of phonons becomes more important.

Figure 4h shows internal energy vs. temperature for different values of pressure. As can be seen from the graph, the internal energy is not zero at zero pressure and zero temperature, but there is some contribution of lattice vibration. The internal energy at zero temperature and zero pressure is 5.62 kJ mol^{-1} , and as the pressure is increased the value of internal energy increases. At higher temperature, all trend lines obtained for different values of pressure have converged at a point.

3.5 Optical properties

The study of optical properties gives information about the behaviour of the material towards the EM radiation. To study these properties, a dense mesh of uniformly distributed k -points is required. The magnitude of the optical properties depends on the polarization of phonons. In the presence of light of suitable wavelength, the electrons make transition from the occupied state to the unoccupied state above the Fermi level.

3.5a Dielectric function: The dielectric function depends upon frequency and is determined by the transition between the valence band and the conduction band. It gives information about the optical response at all photon energies ($\hbar\omega$). The dielectric function is written as

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega), \quad (22)$$

where $\varepsilon_1(\omega)$ represents real part and $\varepsilon_2(\omega)$ represents the imaginary part of the dielectric function $\varepsilon(\omega)$. The imaginary part is calculated using the below equation:

$$\varepsilon_2(\omega) = \left(\frac{4\pi^2 e^2}{m^2 \omega^2} \right) \sum_{i,j} \int \langle i | M | j \rangle^2 f_i (1 - f_j) \times \delta(E_f - E_i - \omega) d^3k, \quad (23)$$

where M is dipole matrix, i and j are the initial and the final states, f_i is the Fermi distribution function for the i th state, and E_i is the energy of the i th state.

The real part of the dielectric function $\varepsilon_1(\omega)$ is extracted from the imaginary part using the Kramer–Kronig equation [59,60]:

$$\varepsilon_1(\omega) = 1 \pm \frac{2}{\pi} P \int_0^\infty \frac{\omega' \varepsilon_2(\omega') d\omega'}{(\omega'^2 - \omega^2)}. \quad (24)$$

Calculated optical parameters as a function of incident energy are shown in figure 5. Figure 5a shows that the threshold energy of the dielectric function occurs at 3.14 eV. The main peak of the imaginary part of the dielectric of magnitude 28.34 (arbitrary units) is located at 5.59 eV. This peak gives the

Figure 5. Calculated optical parameters as a function of incident energy. (a) Real and imaginary parts of dielectric function $\epsilon(\omega)$, (b) refractive index $n(\omega)$ and extinction coefficient $k(\omega)$, (c) optical conductivity $\sigma(\omega)$, (d) electron energy loss function $L(\omega)$, (e) absorption coefficient $\alpha(\omega)$ and (f) reflectivity $R(\omega)$.

optical response caused by the electric dipole transition between conduction and valence band. At higher values of energies, the magnitude of dielectric constant decreases.

The static value of the complex dielectric function is 9.64 (in arbitrary unit) and it reaches the highest peak value of the real part 18.08 at 4.28 eV. Beyond 4.28 eV, $\epsilon_1(\omega)$ starts decreasing with the increase in energy and becomes negative at 7.79 eV; negative value of $\epsilon_1(\omega)$ shows metallic reflectance corresponding to that energy [61].

3.5b Refractive index and extinction coefficient: The refractive index and the extinction coefficient of BAs are

shown in figure 5b. The compounds with high refractive index have high optical nonlinearity. The refractive index increases with energy in the transparency region, and reaches a peak of magnitude 4.501 (arbitrary unit) in the visible region at about 5.26 eV. The extinction coefficient is the highest at 6 eV; which implies that the absorption is prominent at 5.59 eV as the absorption coefficient $\alpha(\omega)$ is related to the extinction coefficient $k(\omega)$ through the following equation:

$$\alpha = \frac{4\pi k}{\lambda}. \quad (25)$$

The refractive index $n(\omega)$ is calculated from the real part of the dielectric function [31]:

$$n(\omega) = \sqrt{\varepsilon_1}. \quad (26)$$

3.5c Optical conductivity: The optical conductivity can be calculated from the dielectric constant using the following equation:

$$\sigma(\omega) = -\frac{i\omega}{4\pi}\varepsilon(\omega). \quad (27)$$

Figure 5c shows the variation of optical conductivity vs. energy. Optical conductivity spectrum of BAs exhibits high conductivity in the energy range of 5.02–6.9 eV with a peak at 5.59 eV that coincides with the peak position of the absorption coefficient. This optical conductivity is mainly caused by the transition from valence bands of As-p states to the conduction bands of B-s state.

3.5d Electron energy loss function: Figure 5d shows variation of electron energy loss function $L(\omega)$ vs. photon energy. The $L(\omega)$ describes the interaction of high electron energy beams with matter. It shows the diverse energy range corresponding to electronic excitation of different orbitals. We find that there is a prominent maximum of energy loss function at 21.75 eV for BAs. The energy loss of the fast traversing electron in the material shows sharp peak in this region. This pronounced maximum of energy loss function corresponds to the plasma frequency or the plasma region. In this plasma region, the valence electron can behave like free particles and take part in collective oscillation. The energy loss curve explains this behaviour very well.

3.5e Optical absorption: The influence of the optical properties on the optoelectronic devices would preferably be known by the optical absorption coefficient α [62–65]. The α is determined by the following equation:

$$\alpha(\omega) = \frac{4\pi k(\omega)}{\lambda}. \quad (28)$$

The spectral dependence of $\alpha(\omega)$ is presented in figure 5e. The absorption is noteworthy at 7.38 eV energy. High absorption and low reflectance of the material in the ultraviolet region makes the material a prominent one for the optoelectronic devices and nonlinear applications.

3.5f Reflectivity: Reflectivity of a material is given by the following equation:

$$R(\omega) = \frac{(n(\omega) - 1)^2 + k(\omega)^2}{(n(\omega) + 1)^2 + k(\omega)^2}. \quad (29)$$

It is one of the most important parameters in linear optical calculations because of its sensitivity towards the combination of $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ [66]. In figure 5f, the maximum reflectivity of BAs is found to be 63% located at 7.6 eV photon energy, which lies in the ultraviolet region.

4. Conclusions

We have performed the first-principles calculations to study fundamental properties of BAs by using the DFT where exchange–correlation functional is solved using the PBEsol-GGA approximation. Our obtained results are compared with the available theoretical and experimental results. Our calculated results are in good agreement. Data related to the direct and indirect band gaps along with total and partial DOS are reported and analysed. Parameters related to the mechanical properties of BAs are calculated and compared with the data available. The thermal properties, which define the stability of the material at various temperatures and pressures, were also analysed and studied. Detailed results related to the optical properties of BAs are also included in this study.

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