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Study of Structural, Electronic, Optical, Mechanical, Thermal, and Thermoelectric Properties of MPSi_3 [$\text{M} = \text{Al}, \text{Ga}, \text{In}$] Semiconductors by DFT Method

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ABSTRACT

In this study, a new semiconducting material, InPSi_3 , has been explored using density functional theory (DFT) calculations, along with an investigation of the unexplored properties of the newly predicted AlPSi_3 and GaPSi_3 semiconductors. The negative formation energy, elastic constants, and positive phonon modes certify the stability of all three compounds. InPSi_3 is an indirect-band-gap semiconductor (1.58 eV), whereas AlPSi_3 and GaPSi_3 are direct band gaps with an E_g of 1.64 and 1.51 eV, respectively. We used DOS to investigate the nature of bonding. Additionally, optical coefficients, including the dielectric constant, refractive index, extinction coefficient, photoconductivity, optical absorption, reflectivity, and loss function, were computed. The mechanical behavior was studied by calculating elastic constants, elastic moduli, and brittleness indices. The thermal parameters, including Debye temperature, melting temperature, thermal conductivity, minimum thermal conductivity, thermal expansion coefficient, and specific heat capacity, have been investigated. The thermoelectric properties, including electrical conductivity (σ/τ), electronic thermal conductivity (K_e/τ), Seebeck coefficient (S), power factor (PF), and figure of merit (ZT), were calculated. The titled materials would be appropriate for individual solar cells or the top portion of tandem solar cells, owing to their appropriate band gap and optical absorption.

1 | Introduction

Semiconductors are essential to our technology-driven world. They are used in many devices, including computers, TVs, iPhones, tablets, and internet infrastructure. The semiconductor industry continually seeks to make electronics faster, smaller, and more efficient, reflecting our desire for better technology. The need for renewable, clean energy is growing as we deplete fossil fuel reserves and pollution rises [1–4]. Solar cells offer a nearly limitless, eco-friendly power source [1, 5, 6]. Today, silicon is used as a substrate in almost 95% of electronic devices, and most solar

cells employ it for its widespread availability, affordability, and safety [7].

Recent efforts have focused on developing new materials or improving existing ones for solar cells. Although silicon is one of the best materials for converting sunlight into energy, it has limitations because its atoms are arranged in a way that creates an indirect band gap, which absorbs longer-wavelength light (approximately 1.1 eV). To make better solar cells, researchers are seeking new silicon-based materials with a direct band gap of a higher value (close to the S. Q. limit) [8] that

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could help solar cells convert sunlight into electricity more efficiently.

The efficiency of silicon-based solar cells has reached the theoretical S-Q limit (33.7%) for single-junction photovoltaic devices [8], despite numerous attempts to enhance their performance [9–15]. Single-gap systems are less efficient across the solar spectrum than multi-gap systems. Tandem solar cells, featuring two junctions, boast a theoretical efficiency of 44% and are constructed from materials with both low- and high-band-gap components, thereby optimizing their ability to absorb incoming solar radiation. With an infinite stack of junctions, the efficiency can reach 65% under one-sun illumination [16].

A combination of Group IV and III-V compounds can form alloys/compounds, which are likely to exhibit a range of direct band gaps. This potential makes them valuable for the development of tandem solar cells. Scientists have studied these alloys both theoretically and experimentally [17]. Alloying of Si with AlP (III-V) or MgS (II-VI) semiconductors modifies the electronic band structure of Si. For example, an indirect band gap value of Ge is 0.7 eV, while the direct band gaps of GaAs and ZnSe are 1.5 and 2.8 eV, respectively [18]. They successfully made $(\text{GaAs})_{0.45}\text{Si}_{0.55}$ using techniques such as rf discharge decomposition and rf sputtering, revealing that it absorbs light with an edge at 1.28 eV [19]. Optical examinations of $(\text{Ge}_2)_x(\text{GaAs})_{1-x}$ have also shown that changing the alloy's composition of x can significantly affect its direct band gap [20–23]. Researchers have used density functional theory to systematically explore 2D BNCx compounds. They found that many of these materials have direct band gaps, making them ideal for absorbing solar light. The BNC₂-type compound is a combination of diamond and C-BN. This compound is harder than diamond and more chemically stable than C [18]. Studies on alloy monolayers such as BNC, BNC₂, and BNC₃ have reported direct band gaps of 1.56, 1.60, and 1.04 eV, respectively [24].

Watkins et al. [25] synthesized the functional AlPSi₃ semiconductor using gas-source molecular beam epitaxy. First-principles simulations validated that AlPSi₃, with Cc symmetry, adopts a diamond-like structure. This detailed analysis enabled the first identification of the chemical environments and preparations of the material's Al-P and Si elements [26]. Subsequently, GaPSi₃ underwent a similar examination, employing comparable methods. The study involved diffraction analysis and optical characterization, revealing single-phase, monocrystalline structures that resemble silicon and exhibit an average diamond-cubic configuration [27]. Researchers have used this method to synthesize AlPSi₃ and AlAsSi₃, and their respective alloys, including $\text{Al}(\text{As}_{1-x}\text{P}_x)\text{Si}_3$, $\text{Al}(\text{As}_{1-x}\text{N}_x)\text{Si}_3$, $\text{Al}(\text{P}_{1-x}\text{N}_x)\text{Si}_3$, $(\text{InP})_y\text{Ge}_{5-2y}$, and $(\text{Al}_{1-x}\text{B}_x)\text{PSi}_3$ [28–30].

The structural, electrical, and optical characteristics of the AlPSi₃ with a Cc structure were thoroughly analyzed. The findings indicate significantly enhanced absorption in the higher-wavelength region compared to the Si absorption band [18]. However, a defect is noted: it exhibits an indirect fundamental band gap of 1.41 eV, whereas its direct band gap is 2.0 eV, which is far from the ideal value for solar cell applications [31]. Yonghui Du et al. studied AlPSi₃ and GaPSi₃ (both Pm-3m and Pm-3n

phases) and found that both have direct or quasi-direct band gaps within the optimum range, as assessed using the HSE06 method. Notably, these materials can absorb a wider range of energies, including both visible and ultraviolet light. Previous research on AlPSi₃ and GaPSi₃ encouraged us to consider InPSi₃ as a potential target material. The band gap values for AlPSi₃ (1.75 eV) and GaPSi₃ (1.71 eV) helped us to expect a smaller band gap (closer to the S.Q. limit –1.43 eV) for InPSi₃ than that of AlPSi₃ and GaPSi₃, owing to the lower position in a column of the periodic table. In addition, limited information (only electronic and optical absorption) of AlPSi₃ and GaPSi₃ is not enough for practical use, which also urges us to determine the elastic and thermal properties of previously known compounds (AlPSi₃ and GaPSi₃). Moreover, some reports on Al-, Ga-, and Si-based materials also motivate us to select the titled materials. For example, Beenaben et al. [32] have studied the half-Heusler alloys TiAgZ (Z = Al, Ga, In) and reported their thermoelectric properties. Beenaben et al. [33, 34] have also studied Si-based alloys, such as TaPtSi and MnNiSi, and studied their thermoelectric properties. Yin et al. [35] reported a high ZT value of 1.48 for $\text{In}_4\text{Se}_{3-\delta}$ ($\delta = 0.65$), indicating very good performance as a thermoelectric material.

Therefore, AlPSi₃, GaPSi₃, and InPSi₃ have been selected for this research project, in which we conducted a first-of-its-kind study of InPSi₃ and explored the physical properties of AlPSi₃ and GaPSi₃ that have not been explored before. To make the study comprehensive, we will also revisit the properties of AlPSi₃ and GaPSi₃ semiconductors.

2 | Computational Techniques

To calculate the physical attributes of the MPSi₃ [M = Al, Ga, In] semiconductors, the DFT [36, 37] was accomplished in the Cambridge Serial Total Energy Package (CASTEP) code [38]. The structural and thermo-mechanical properties were calculated using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional [39], where the electron-ion interactions were treated by ultra-soft pseudopotentials. In addition, norm-conserving pseudo-potential [40] and hybrid (HSE-06) methods were employed to determine the electronic and optical properties. The valence electron configurations Al (3s² 3p¹), Ga (3d¹⁰ 4s² 4p¹), In (4d¹⁰ 5s² 5p¹), P (3s² 3p³), and Si (3s² 3p²) were used. Some parameters were fixed for the crystal optimization of the first Brillouin Zone (BZ), such that the plane wave cutoff energy is 600 eV for both exchange-correlation approximation with the grid of k -point $4 \times 8 \times 5$ in the GGA-PBE exchange-correlation functional and the grid of k -point $2 \times 4 \times 2$ in the HSE06 hybrid approach [41]. The structures were minimized with the energy by some factors: the self-consistent equilibrium of the total energy was 5×10^{-6} eV per atom, the tolerance for the self-consistent field was 5×10^{-6} eV per atom, the highest force was 0.01 eV/Å, and the maximum stress was 0.02 GPa. The cutoff and k -points were selected by converging the structure with these settings, yielding the lowest total energy of the unit cell (optimized cell). The mechanical behavior was investigated by computing the elastic constants using the stress-strain approach, which was further used to compute the elastic moduli.

TABLE 1 | Lattice constants, Final volume, and Formation energy of AlPSi₃, GaPSi₃, and InPSi₃.

Parameters	AlPSi ₃		GaPSi ₃	InPSi ₃
a (Å)	8.611	8.621 [17]	8.624	8.833
b (Å)	3.858	3.863 [17]	3.841	3.945
c (Å)	6.752	6.758 [17]	6.741	7.087
Final Volume (Å ³)	217.818		216.611	239.883
Formation Energy (eV)	−0.261		−0.737	−0.108

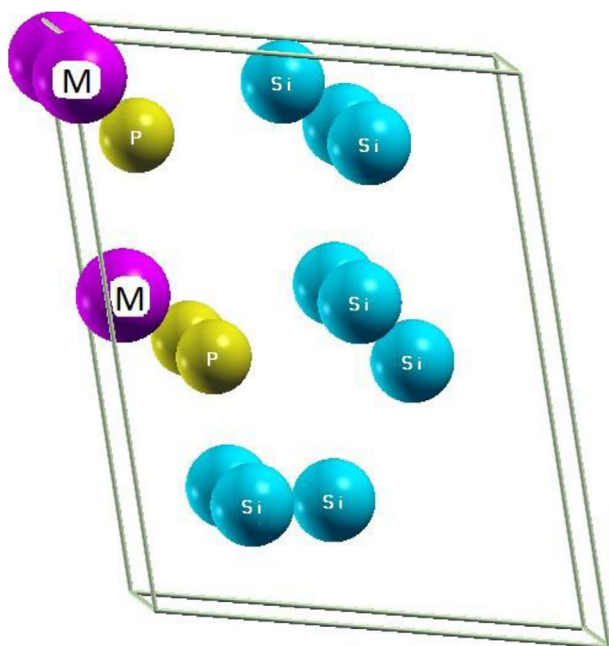


FIGURE 1 | Unit cell of AlPSi₃/GaPSi₃/ InPSi₃.

3 | Results and Discussion

3.1 | Structural Properties

MPSi₃ [M = Al, Ga, In] crystallized in a monoclinic system with space group of Pm-a, as shown in Figure 1. The atomic positions included the following: Al (0.932, 0.000, 0.016), Al (0.537, 0.500, 0.061), P (0.456, 0.000, 0.218), P (0.822, 0.500, 0.147), Si (0.855, 0.000, 0.640), Si (0.462, 0.500, 0.685), Si (0.200, 0.000, 0.253), Si (0.937, 0.500, 0.492), Si (0.573, 0.000, 0.563), and Si (0.205, 0.500, 0.460 [32-complementary table-S1 from Y. Du; then the reference will be-17]. The unit cell contains a total of 10 atoms. In particular, 2 P atoms, 6 Si atoms, and 2 Al/Ga/In atoms are present. The obtained lattice constants and volume of the optimized cell are shown in Table 1. The lattice parameters of AlPSi₃ matched very well (deviation around 0.1%) with those reported in [17].

Among the studied compounds, AlPSi₃ and GaPSi₃ were known, and we predicted InPSi₃ as a promising candidate for solar cell technology in this study. In predicting materials, stability checks are a must, and we have conducted this study by calculating formation energies, phonon dispersion curves (PDC), and elastic constants. Formation energy has been computed using the widely used formula: $\Delta = \frac{E_{\text{Total}} - E_{\text{Isolated}}}{\text{Number of total atoms}}$ and given in Table 1. The

formation energy of the three titled compounds yields a negative value, confirming their stability [42]. It should be noted that the stability of AlPSi₃ and GaPSi₃ has been confirmed in a previous study [17]. The negative formation energy supports our results that these two, along with the newly predicted InPSi₃, could be synthesized.

In support of this result, we also calculated the PDC, shown in Figure 2, in which no imaginary phonon frequencies are found. The phonon dispersion, without imaginary frequencies, further certifies the stability in the dynamics of the three compounds studied herein. Finally, the mechanical stability was also examined and presented in Section 3.4.1. The titled compounds have satisfied all the stability criteria; hence, as with previously known AlPSi₃ and GaPSi₃ tandem solar cell materials, a new InPSi₃ has been successfully predicted here and is expected to be a potential application in solar cell technology.

The PDC of the compounds also infers some additional features. For example, the studied compounds have 10 atoms per unit cell. Thus, a total of 30 curves are present in the figure. The lowest 03 are acoustic; the rest, 27, are known as optical modes. The dispersion of transverse acoustic modes reduces from Al to Ga to In, i.e., from lighter to heavier elements. The reduced dispersion of transverse acoustic modes indicates phonon localization, resulting in a reduced group velocity for InPSi₃, followed by AlPSi₃ and GaPSi₃. Another essential feature lies in the hybridized region between the aural and optical branches (in the lower optical modes). The hybridization, or overlap, of the acoustic and lower parts of optical modes contributes to the non-conducting properties of heat. Thus, the more branches hybridized, the greater the thermal resistance due to increased phonon scattering; consequently, the solids exhibit lower lattice thermal conductivity [43, 44]. Figure 2 reveals the strongest coupling for InPSi₃, followed by AlPSi₃ and GaPSi₃. Thus, the lowest lattice thermal conductivity is expected for InPSi₃, followed by AlPSi₃ and GaPSi₃, as shown in Table 6.

3.2 | Electronic Properties

3.2.1 | Band Structure and Carrier Effective Masses

Understanding the electronic band structure helps to understand optical characteristics. An electronic band diagram controls the optical and transport properties of solids, including the optical bands and electron transport. The efficiency of energy conversion in photovoltaic systems is significantly influenced by the band gap. The material's band gap lies within the S-Q limit of 1.1–1.8 eV, while the conversion efficiency ranges from 26.86% to

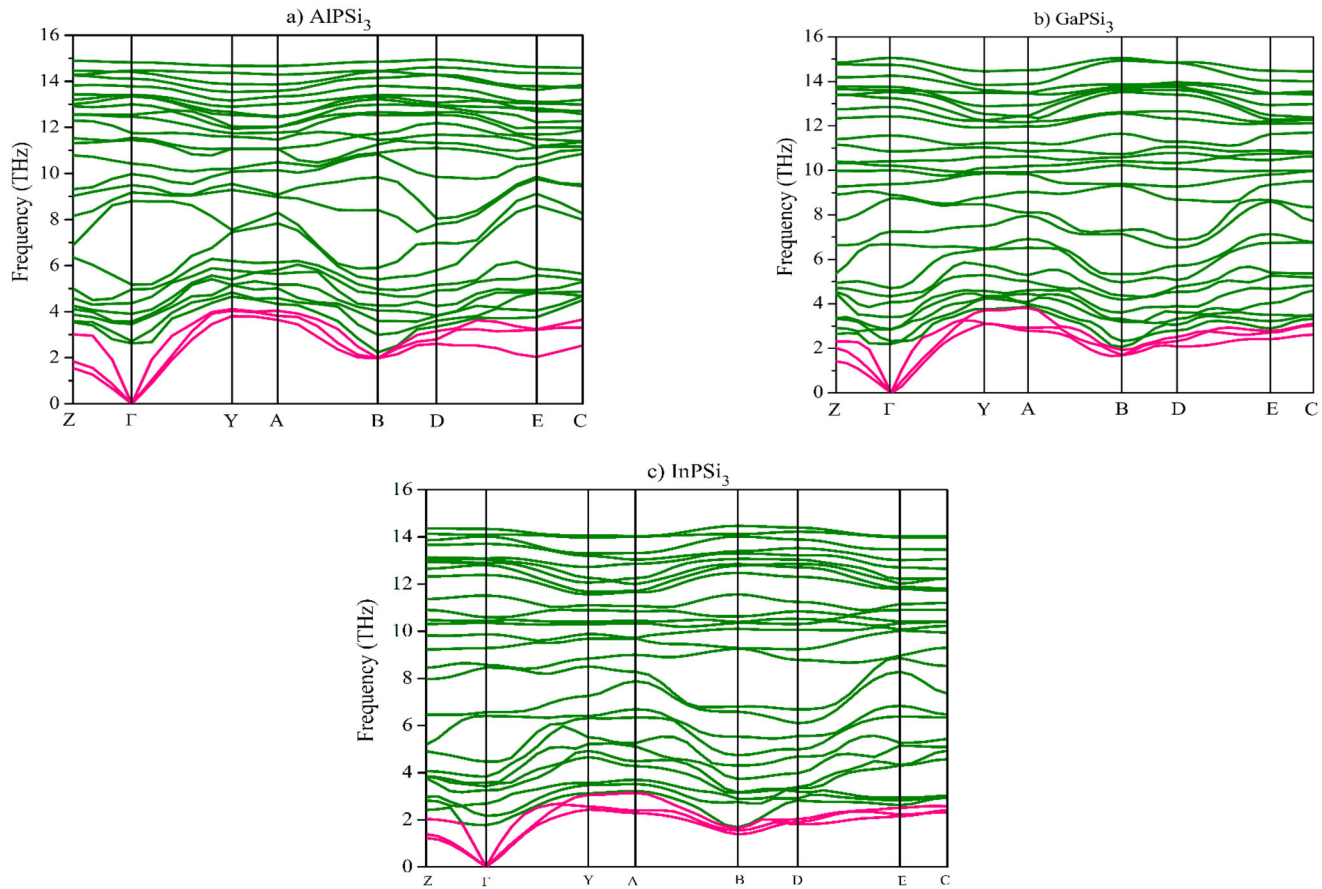


FIGURE 2 | Dispersion of phonon (a) AlPSi₃, (b) GaPSi₃, and (c) InPSi₃.

TABLE 2 | Calculated electronic band gap of MPSi₃ [M = Al, Ga, In].

Compound	GGA-PBE	HSE-06	Reference	m_e^*/m_0	m_h^*/m_0
AlPSi ₃	1.10 eV1.12 eV	1.643 eV1.75 eV	This workRef. [17]	0.0172	0.146
GaPSi ₃	1.07 eV1.07 eV	1.514 eV1.71 eV	This workRef. [17]	0.0160	0.099
InPSi ₃	0.785 eV	1.583 eV	This work	0.0169	0.218

33.16% [45]. Band structures of AlPSi₃, GaPSi₃, and InPSi₃ are shown in Figure 3, confirming that they are semiconducting. In addition, AlPSi₃ and GaPSi₃ demonstrate a direct band gap nature at the D—point in both GGA-PBE and HSE-06, displayed in Figure 3. The herein predicted compound, InPSi₃, exhibits an indirect band gap for both GGA-PBE and HSE-06 methods; the minimum conduction band is found at the D point. At the same time, the maximum valence is seen at the Γ point. The obtained band gaps are given in Table 2. From this, it is evident that the values obtained with GGA-PBE are lower than those obtained with HSE-06. Usually, the functional GGA-PBE underestimates band gaps [46, 47], whereas HSE-06 provides a more accurate estimate of band gaps for semiconductors [17]. The optimal range for the electronic band gap of our titled compounds is 1.1–1.8 eV, which aligns with the Shockley-Queisser limit. The energy gaps of AlPSi₃, GaPSi₃, and InPSi₃ are 1.64, 1.51, and 1.58 eV, respectively, as calculated using HSE-06, as shown in Table 2. Consequently, these materials are well-suited for the upper cell of tandem-type solar cells, given that the ideal band gap for the top cell

in two-junction tandem solar cells is between 1.5 and 2.0 eV [48]. However, the calculated band gap values for AlPSi₃ and GaPSi₃ differ slightly from the reported values [17] (see Table 2) due to differences in computational codes and k-point sampling. The values calculated using GGA-PBE agree very well with the reported values, but those obtained with HSE-06 differ slightly larger due to a mismatch in the k-point grids. The electronic band gaps of MPSi₃ [M = Al, Ga, In] are slightly lower than those of similar 113 compounds XPbI₃ (X = Al, Ga, In, Tl) [49]. The authors concluded that these materials [XPbI₃ (X = Al, Ga, In, Tl)] have strong potential for solar cell and photovoltaic applications. Thus, a similar application is also expected for the titled solids.

The effective masses of electrons (m_e^*/m_0) for MPSi₃ (M = Al, Ga, In) are found to be 0.0172, 0.0160, and 0.0169, respectively, indicating very light electrons. In contrast, the hole effective masses (m_h^*/m_0) are higher, with values of 0.146, 0.099, and 0.218, as shown in Table 2. This difference suggests that elec-

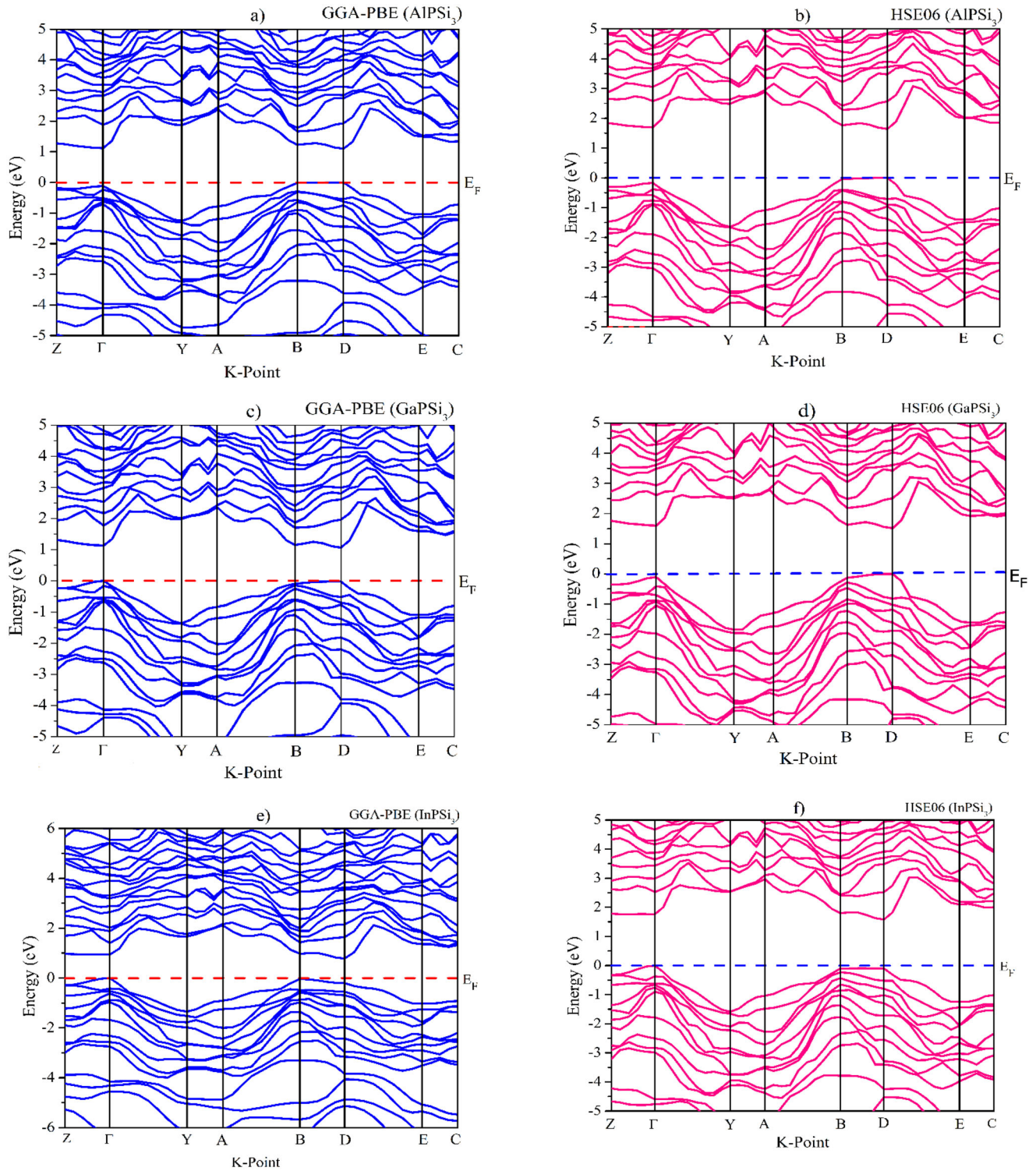


FIGURE 3 | Band diagram of AlPSi₃, GaPSi₃ and InPSi₃ by using GGA-PBE (blue line) and HSE-06 (Pink line).

trons are likely to have higher mobility [50] than holes due to the more dispersive nature of the conduction bands. The curvature of the bands reveals the carrier motion, which can be obtained by computing the effective masses [51]. Among the studied compounds, the Ga-based compounds show comparatively lower effective masses for both carriers, indicating more favorable transport characteristics. Overall, the effective mass of electrons (low) and holes (moderate) revealed the

suitability of these in optoelectronic and photovoltaic applications.

3.2.2 | Density of States

Figure 4 shows the total and partial density of states (DOS) from -5 eV to +5 eV. Each compound exhibits a distinct gap, confirming the semiconducting nature of the materials.

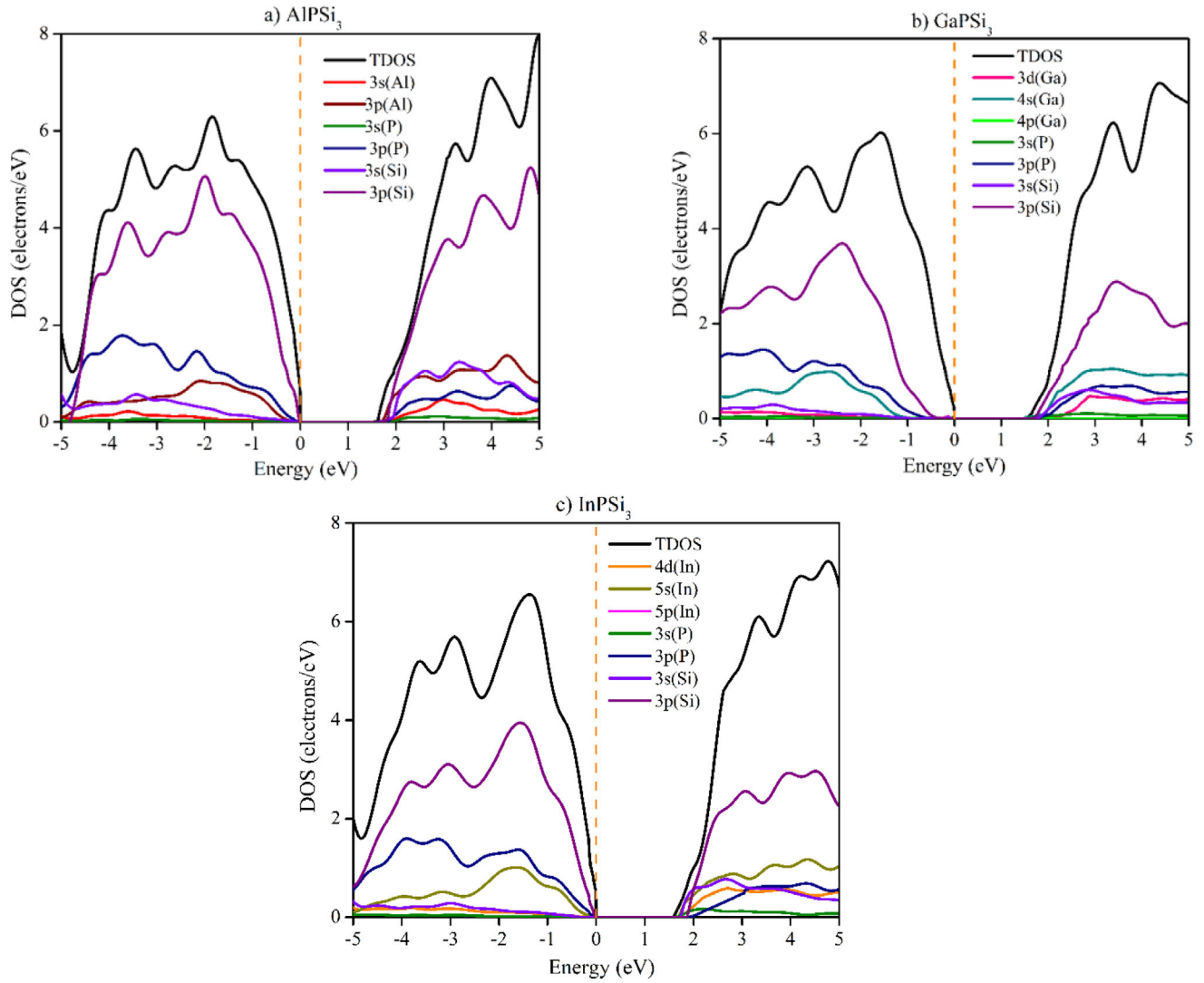


FIGURE 4 | Total and Partial DOS (PDOS) of (a) AlPSi₃, (b) GaPSi₃, and (c) InPSi₃.

The Fermi level position closer to the valence band indicates a P-type semiconductor [52]. The PDOS emphasizes the influence of specific atomic orbitals or components on the total DOS, enhancing a deep understanding of bonding and electronic configurations. Figure 4 indicates that the primary contribution arises from the Si-3p state in both the valence and conduction bands. A significant hybridization is evident between the Si-3p and P-3p states, with a lesser contribution from the M-3p states across all three compounds. Consequently, covalent bonding is anticipated among the M-*p*, P-*p*, and Si-*p* states.

3.3 | Optical Properties

Optical devices operate based on the material's response to light, which in turn affects their performance. The optical properties are examined through the relationship between the optical absorption of incoming light and the transition of charge carriers from the valence to the conduction band [53].

The optical phenomena of these three compounds are measured as a function of photon energy, with polarization vectors [001]

and [010], up to 20 eV. It is noted that the dielectric function (ω) = $\epsilon_1(\omega)$ + $i\epsilon_2(\omega)$ is used to determine the optical parameters, where the dielectric function is frequency-dependent [54]. The real (RDF) and imaginary (IDF) parts of the dielectric functions are $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$, respectively, where ω is the angular frequency, calculated using the Kohn–Shams [55] and Kramers–Kronig [56] equations. Electrical polarization is expressed by the IDF, and the absorption of incident light energy is revealed by the IDF. The dielectric constant of the real part, which is denoted as $\epsilon_1(0)$, depends on the band gap. At zero frequency, it is called the static dielectric constant, as shown in Figure 5a. A greater static dielectric constant indicates a narrower band gap, as depicted in Table 3 [57, 58].

The $\epsilon_2(\omega)$ is closely related to the photon absorption. It measures the energy absorbed by the material from incident light. Electronic excitations are generated by optical absorption, an important process to understand the optical properties of materials. Peaks in $\epsilon_2(\omega)$ are usually generated by interband shifts, where electrons move within their band. The peak energy is defined as the energy difference between the initial and final states of the transition [59]. In Figure 5b, GaPSi₃ exhibits the highest peak in

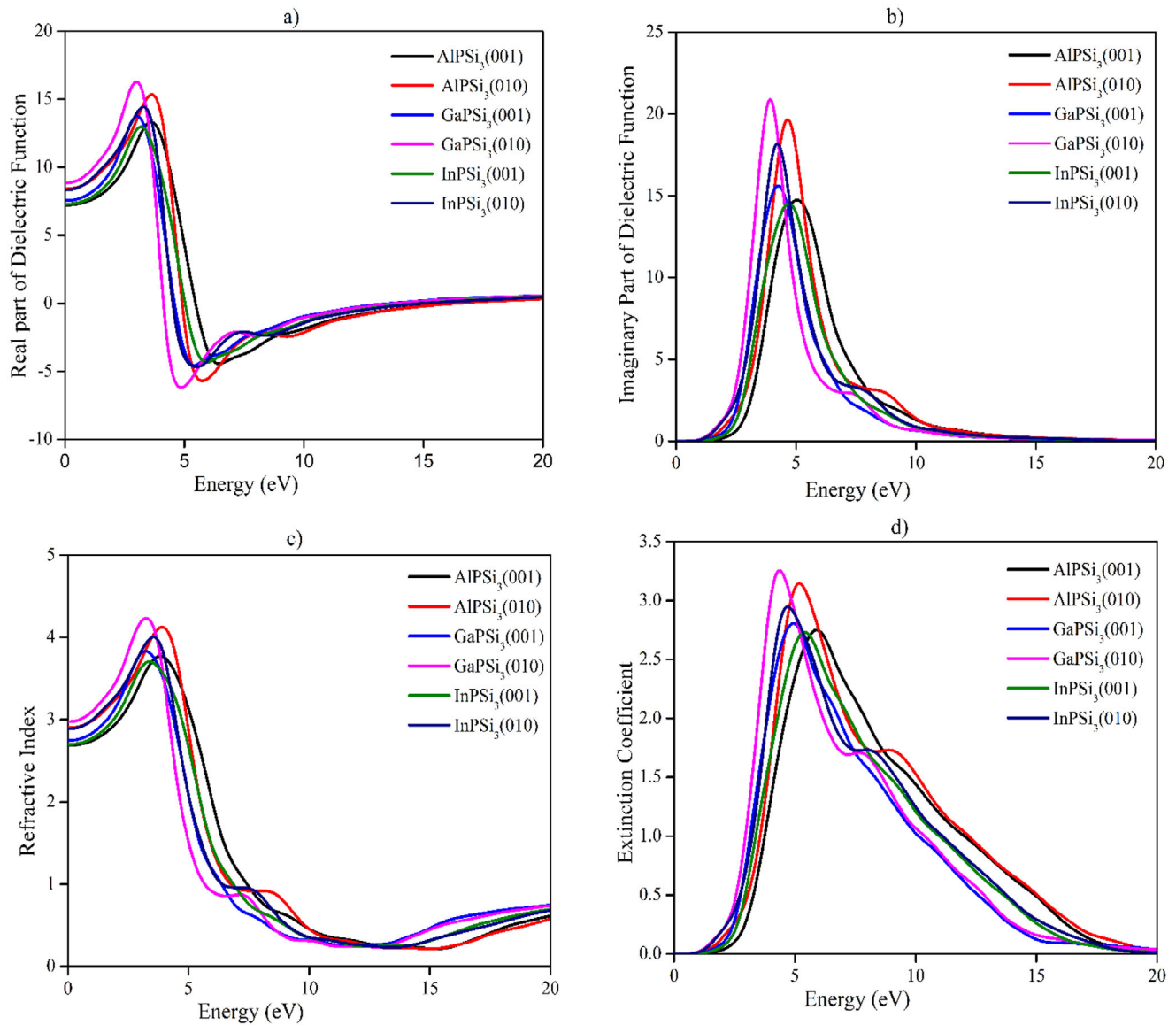


FIGURE 5 | (a) Real part of the dielectric function, (b) Imaginary part of the dielectric function, (c) Refractive index, and (d) Extinction coefficient of AlPSi₃, GaPSi₃, and InPSi₃.

TABLE 3 | Some critical optical parameters.

Compound	direction	$\epsilon_1(0)$	$n(0)$	$R(0)$
AlPSi ₃	(001)	7.266	2.692	0.210
	(010)	8.372	2.894	0.237
GaPSi ₃	(001)	7.552	2.741	0.218
	(010)	8.814	2.983	0.247
InPSi ₃	(001)	7.266	2.700	0.210
	(010)	8.372	2.894	0.236

the [010] direction, a value similar to that found in the absorption diagram (Figure 6a) for GaPSi₃ at [010] direction, which is linked with a narrower electronic band gap of GaPSi₃ (1.51 eV).

The absorption coefficient spectra began at specific values near the band gap in each case, as illustrated in Figure 6a. Direct-band-gap materials exhibit higher optical absorption in the shorter-wavelength region of visible light [60]. The highest peaks are observed at about 3–7 eV, but they originate near 1.5 eV, which defines the absorption edge in the visible spectrum. As seen, the peak of highest absorption [at 4.68 eV], a value reflected in the imaginary portion of the dielectric function as in Figure 5b, is found for GaPSi₃ in the [010] direction, which also starts in the greater wavelength area of the visual range, certifying the best absorption capability of this one among the studied compounds. The highest absorption peak of GaPSi₃ in the [010] direction arises from strong anisotropic interband electronic transitions associated with its anisotropic electronic band structure. However, the peaks exhibited by the studied compounds are quite similar; they differ only slightly in peak position and height, due to differences in energy band gap:

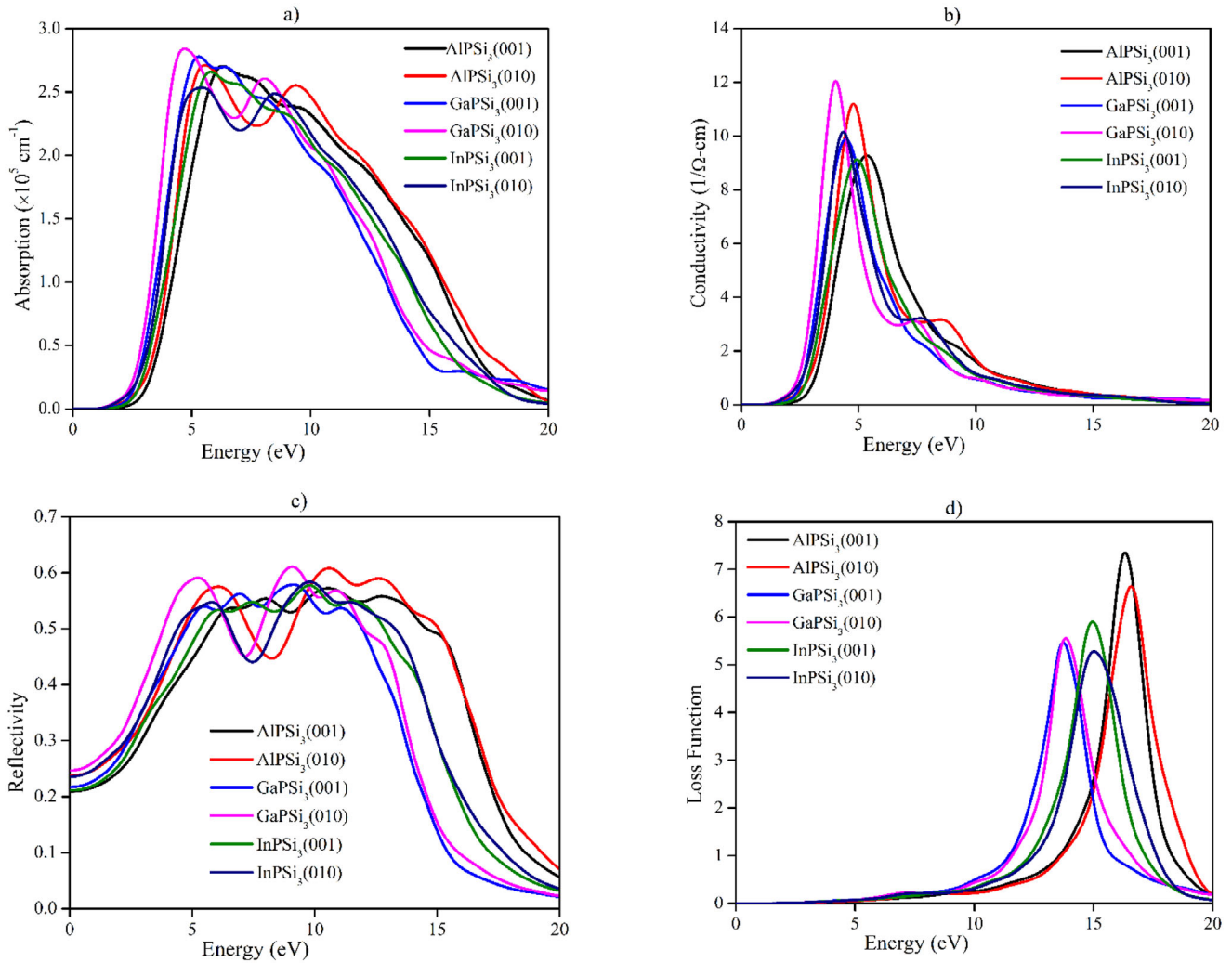


FIGURE 6 | (a) Absorption, (b) Conductivity, (c) Reflectivity, and (d) Loss function of AlPSi₃, GaPSi₃, and InPSi₃.

the smaller the band gap, the higher the absorption peaks [e.g., GaPSi₃]. The compounds show strong absorption [$>10^5$ cm⁻¹] in the visible region, and band gaps are within 1.514 to 1.75 eV, signifying promising application as top-cell absorbers in tandem solar cells and enhanced light harvesting in the visible range.

The absorption of electromagnetic waves (photons) enhances conductivity. Optical conductivity is determined by the density of free carriers and their mobility. Optical conductivity is similar to electrical conductivity, enabling these materials to be used in the fabrication of optoelectronic devices. In the [010] direction of GaPSi₃, the highest peak of conductivity is observed at 4.03 eV, reaching a value of 12.068 (1/Ω-cm), shown in Figure 6b. Additional peaks for the proposed materials are situated in the ultraviolet region. It is noteworthy that all compounds exhibit insulating behavior above 20 eV. It is confirmed that these materials are semiconductors because they do not exhibit photoconductivity at zero photon energy.

The quantity of incoming light reflected by the surface of semiconducting materials is referred to as optical reflectivity, *R*. These components are used as coating materials where

absorption is not required. Figure 6a,c presents a comparative illustration indicating that absorption is inversely proportional to optical reflectivity. A low reflectivity value is expected for absorbing materials. As is evident, the titled materials exhibit low reflectivity in the low-energy region, which also supports our prediction that the studied materials could be used as an absorbing layer in solar cell technology.

The optical loss function describes how energy is lost by electrons as they pass through a compound. The loss function remains minimal within the range of 2.5 eV. The loss function is at its minimum from 2.5 eV to nearly 10 eV. As illustrated in Figure 6d, the optical loss increases rapidly beyond 10 eV, reaching a maximum at 16.32 eV. The TiAgZ (Z = Al, Ga, and In) compounds also exhibit a maximum energy loss of 20.9 eV [61]. Given its band gap, our compound exhibits excellent absorption with minimal loss.

These materials will be used in tandem solar cells, which leverage their absorption properties [62]. Finally, the figure shows significant absorption in the visible and ultraviolet regions, as indicated by the imaginary dielectric constant, extinction coefficient, and absorption coefficient.

TABLE 4 | Elastic constants C_{ij} of MPSi₃ [M = Al, Ga, In].

Elastic constant	AlPSi ₃	GaPSi ₃	InPSi ₃
C_{11} (GPa)	167.18	170.37	144.05
C_{22} (GPa)	148.41	149.48	127.14
C_{33} (GPa)	138.05	140.65	123.95
C_{44} (GPa)	44.27	51.07	37.94
C_{55} (GPa)	35.22	40.05	28.79
C_{66} (GPa)	43.44	45.88	38.14
C_{12} (GPa)	30.84	28.06	25.65
C_{13} (GPa)	42.14	38.52	36.73
C_{15} (GPa)	−1.34	−0.61	−0.44
C_{23} (GPa)	40.47	38.24	37.24
C_{25} (GPa)	−5.64	−5.83	−3.46
C_{35} (GPa)	7.59	8.53	8.77
C_{46} (GPa)	−10.41	−10.41	−9.85

3.4 | Mechanical Properties

3.4.1 | Elastic Properties

Studying the mechanical properties of semiconducting materials used in solar cell technology is crucial for assessing their sustainability under environmental conditions, including wind, hail, and temperature variations. By examining these properties, researchers can identify potential weaknesses and develop strategies to enhance the durability and reliability of solar cells. This ensures they can withstand the challenges posed by various climates and weather conditions. This knowledge is essential for advancing solar technology and promoting its viability as a sustainable energy source. In this section, we have examined the elastic constants and moduli of the materials in question. The elastic tensors C_{ij} obtained from the studied materials are presented in Table 4 and are commonly used to assess mechanical stability and anisotropic bonding characteristics.

The C_{11} , C_{22} , C_{33} , C_{44} , C_{55} , C_{66} , C_{12} , C_{13} , C_{15} , C_{23} , C_{25} , C_{35} , and C_{46} are the thirteen (13) independent elastic constants. The material's stiffness value is expressed by C_{11} , C_{22} and C_{33} when uniaxial tension is employed in the direction of x , y , and z , respectively. The measurement of the shear elastic modulus in the y –direction within the z –plane, in the z –direction within the x –plane and in the z –direction within the y –plane, is usually stated by C_{44} , C_{55} , and C_{66} , respectively. This is the first-time calculation of the elastic constants of AlPSi₃, GaPSi₃, and InPSi₃. Here, the values of C_{11} , C_{22} and C_{33} , in this case, are significantly higher than the values of C_{44} , C_{55} , C_{66} , C_{12} , C_{13} , C_{15} , C_{23} , C_{25} , C_{35} , and C_{46} indicating that greater resistance to unidirectional compressions than to shear deformation [63].

For the monoclinic system, the stability conditions based on the elastic constant C_{ij} are given below [64]:

$$C_{ij} > 0,$$

$$i = 1, 2, 3, 4, 5, 6 \quad [C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] > 0,$$

$$(C_{33} C_{55} - C_{35}^2) > 0,$$

$$(C_{44} C_{66} - C_{46}^2) > 0, (C_{22} + C_{33} - C_{23}) > 0,$$

$$[C_{22} (C_{33} C_{55} - C_{35}^2) + 2C_{23} C_{25} C_{35} - C_{23}^2 C_{55} - C_{25}^2 C_{35}] > 0,$$

$$2[C_{15} C_{25} (C_{33} C_{12} - C_{13} C_{23}) + C_{15} C_{35} (C_{22} C_{13} - C_{12} C_{23}) + C_{25} C_{35} (C_{11} C_{23} - C_{12} C_{13})] - [C_{15}^2 (C_{22} C_{33} - C_{23}^2) + C_{25}^2 (C_{11} C_{33} - C_{13}^2) + C_{35}^2 (C_{11} C_{22} - C_{12}^2)] + C_{55} g > 0$$

$$\text{where } g = C_{11} C_{22} C_{33} - C_{11} C_{23}^2 - C_{22} C_{13}^2 - C_{33} C_{12}^2 + C_{12} C_{13} C_{23}$$

Table 4 clearly shows that the titled materials satisfy the stability conditions. Thus, they are considered stable. Though some of the elastic constants are negative, similar to other compounds belonging to the monoclinic systems [65].

The Hill approximations represent the mean of the Voigt and Reuss estimations for polycrystalline behavior. The bulk modulus (B) and shear modulus (G) were estimated by Hill approximation as follows [66, 67]:

$$B_H = \frac{1}{2} (B_V + B_R), \quad G_H = \frac{1}{2} (G_V + G_R) \quad (1)$$

The values of Voigt and Reuss for B and G are B_V , B_R and G_V , G_R . The bulk modulus demonstrates how solids can withstand compression. The resistance to deformation or changes in shape under shearing stress is represented by G . The rigidity of the materials increases with their shear modulus [68].

The Y obtained from DFT calculations is 97.59 for InPSi₃, 121.80 for GaPSi₃, and 113.82 for AlPSi₃. We verified the same result using the following equation:

$$Y = \frac{9BG}{3B + G} \quad (2)$$

The stiffness of solids is measured by the Young's modulus, Y . It is also known as resistance to longitudinal tension. A material is considered stiffer when its Young's modulus is greater. Based on Young's modulus values, GaPSi₃ is identified as the stiffest material, while InPSi₃ is the least stiff. The Poisson's ratio is expressed as follows:

$$\nu = \frac{3B - 2G}{6B + 2G} \quad (3)$$

Pugh's ratio refers to the relationship between G and B , given by the formula (G/B) . Materials are classified as brittle [$G/B > 0.57$] and as ductile [$G/B < 0.57$]. According to Table 5, MPSi₃ [M = Al, Ga, In] are classified as a brittle material [69].

The Poisson's ratio (ν) is utilized to evaluate the brittleness and flexibility of the studied compounds. The crucial value 0.26 determines whether a material is brittle (lower than 0.26) or ductile (greater than 0.26). From Table 5, we see that the Poisson's ratios are below 0.26, indicating the brittleness of these materials [70, 71].

TABLE 5 | Elastic moduli of MPSi₃ [M = Al, Ga, In]

Compounds	AlPSi ₃	GaPSi ₃	InPSi ₃
Y (GPa)	113.83	121.81	97.59
B (GPa)	75.49	74.33	65.93
G (GPa)	45.58	49.64	38.94
Pugh's ratio (G/B)	0.60	0.67	0.59
Poisson's ratio, ν	0.25	0.23	0.25
Cauchy pressure (GPa)	-13.43	-23.01	-12.29
H_{Chen} (GPa)	7.35	9.24	6.20
H_{Tian} (GPa)	7.75	9.23	6.76
H_{Miao} (GPa)	7.59	8.91	6.51
A_B	0.16	0.17	0.17
A_G	3.70	2.96	4.46
A^U	0.38%	0.31%	0.47%

The Cauchy pressure (C_{12} - C_{44}) was used to characterize the chemical bonding in the materials, as suggested by Pettifor. A positive Cauchy pressure (CP) indicates the presence of metallic bonding (and ductile behavior). In contrast, a negative CP designates directional covalent bonding (brittleness character) [72]. Significant negative values (shown in Table 5) indicate the brittle nature of these solids.

The hardness parameters of MPSi₃ [M = Al, Ga, In] were calculated using the following formulae [73–75]:

$$H_{\text{Chen}} = 2 \left[\left(\frac{G}{B} \right)^2 G \right]^{0.585} - 3 \quad (4)$$

$$H_{\text{Tian}} = 0.92 \left(\frac{G}{B} \right)^{1.137} G^{0.708} \quad (5)$$

$$H_{\text{Miao}} = \frac{(1 - 2\nu)Y}{6(1 + \nu)} \quad (6)$$

The calculated results, shown in Table 5, are quite low, indicating the soft nature of the studied materials. We calculated the hardness of three materials using three different approaches, as defined by Equations (7)–(9). The results for AlPSi₃ ($H_{\text{Chen}} = 7.35$ GPa, $H_{\text{Tian}} = 7.75$ GPa, and $H_{\text{Miao}} = 7.59$ GPa), GaPSi₃ ($H_{\text{Chen}} = 9.24$ GPa, $H_{\text{Tian}} = 9.23$ GPa, and $H_{\text{Miao}} = 8.91$ GPa), and InPSi₃ ($H_{\text{Chen}} = 6.20$ GPa, $H_{\text{Tian}} = 6.76$ GPa, and $H_{\text{Miao}} = 6.51$ GPa) are in line and agree well with each other. Among the three materials, GaPSi₃ is the hardest compound. Hardness also indirectly indicates the mechanical stability of materials, which is advantageous for practical applications, particularly in optoelectronic and photovoltaic devices, where material structural integrity is important during fabrication and operation. The elastic constant, C_{44} , and shear modulus (G) are expected to be better hardness predictors among the elastic constants and moduli [76, 77]. The rankings of C_{44} , G , H_{Chen} , H_{Tian} , and H_{Miao} are similar across the three studied materials.

3.4.2 | Anisotropy

Elastic constants C_{ij} are usually used to express anisotropic characters of binding and structural stability. The modulus of shear (G) and Young's (Y) are related to those elastic constants [78]. The anisotropy percentage in compression and shear is used to assess the elastic anisotropy of poly-crystalline solids [79], which has been calculated as follows:

$$A_B = \frac{B_V - B_R}{B_V + B_R} \times 100\% \quad (7)$$

and

$$A_G = \frac{G_V - G_R}{G_V + G_R} \times 100\% \quad (8)$$

where B and G are the bulk and shear modulus, respectively, while their indices V and R symbolize the Voigt and Reuss limits. Both A_B and A_G values are zero; indicating that the materials are completely isotropic. However, when the values are above zero, the materials are anisotropic and demonstrate increasing anisotropy with higher values [68]. Table 5 shows that the materials AlPSi₃, GaPSi₃, and InPSi₃ are anisotropic.

A^U , a universal anisotropy index that was suggested by Ranganathan and Ostoja-Starzewski [80], is also calculated by this formula,

$$A^U = 5 \frac{G_V}{G_R} + \frac{B_V}{B_R} - 6 \quad (9)$$

For isotropic crystals, $A^U = 0$. A value $A^U > 0$ indicates that the material is anisotropic. The obtained values are presented in Table 5. AlPSi₃ ($A^U = 0.38$), GaPSi₃ ($A^U = 0.31$) and InPSi₃ ($A^U = 0.47$) describes the InPSi₃ is more anisotropic than two other compounds.

3.5 | Thermal Properties

In a crystal that where can be created highest vibrational frequency is defined by the Debye temperature (θ_D). Many parameters depend on the Debye temperature (θ_D), including the melting point, thermal expansion coefficient (TEC), specific heat, lattice vibrations, thermal conductivity, etc [80, 81]. The correlation between the Debye temperature (θ_D) and the mean sound wave speed (v_m) can be found by [80],

$$\theta_D = \frac{h}{K_B} v_m \left[\frac{3n N_A \rho}{4\pi M} \right]^{\frac{1}{3}} \quad (10)$$

The formula for calculating the speed of sound waves is [80],

$$v_m = \left[\frac{1}{3} (2v_T^{-3} + v_L^{-3}) \right]^{-\frac{1}{3}} \quad (11)$$

The velocity of a longitudinal wave in an elastic medium (v_L) and the velocity of a transverse wave in an elastic medium (v_T) in this

TABLE 6 | The Mass (M in Kg), Density (ρ in kg/m³), Longitudinal sound velocity (v_L in m/s), Transverse sound velocity (v_T in m/s), Average sound velocity (v_m in m/s), Debye temperature (Θ_D in K), Melting temperature (T_m in K), Grüneisen parameter (γ_G), Minimum thermal conductivity (K_{min} in W/mK), and Lattice thermal conductivity (K_{ph} in W/mK).

Phase	M (kg)	ρ (kg/m ³)	v_L (m/s)	v_T (m/s)	v_m (m/s)	Θ_D (K)	T_m (K)	γ_G	K_{min} (W/mK)	K_{ph} (W/mK)
AlPSi ₃	0.1422	2.168	7928	4580	5090	539	1270	1.49	1.80	13.2
GaPSi ₃	0.1849	2.837	7038	4183	4631	492	1287	1.39	1.64	15.0
InPSi ₃	0.2300	3.204	6065	3486	3870	397	1158	1.52	1.02	08.5

instance are determined as [82],

$$v_L = \left[\frac{3B + 4G}{3\rho} \right]^{\frac{1}{2}} \quad (12)$$

$$v_T = \left[\frac{G}{\rho} \right]^{\frac{1}{2}} \quad (13)$$

The average sound velocity, v_m can be used to obtain a numerical estimate of Θ_D using the Equation (10). Higher magnitude v_m are correlated with greater values Θ_D . The Θ_D of InPSi₃ is $\Theta_D = 397$ K when $v_m = 3841 \text{ ms}^{-1}$; while for GaPSi₃, it is $\Theta_D = 492$ K with $v_m = 4605 \text{ ms}^{-1}$; and for AlPSi₃, it is $\Theta_D = 539$ K with $v_m = 5054 \text{ ms}^{-1}$. The Debye temperature, Θ_D , is also subject to the molecular weight (M). As molecular weight increases, the density of the solid increases; consequently, the Debye temperature decreases [83], as shown in Table 6.

Melting temperature (T_m) is a vital characteristic property for the selection of high-temperature application materials, which is estimated as follows:

$$T_m = 354 + 4.5 \frac{2(C_{11} + C_{33})}{3} \quad (14)$$

The resulting T_m are given in Table 6; the melting point of GaPSi₃ is 1287 K, the highest among the materials due to its largest elastic moduli [84]. This high temperature makes the material more stable and better able to resist thermal decomposition than the other two materials mentioned.

Thermal conductivity defines how effectively a solid transfers heat, which depends on the velocity of its acoustic waves. We can also describe thermal conductivity in terms of lattice vibrations in solids at a specific temperature ($T = 300$ K). A higher lattice thermal conductivity in a material makes it suitable for use as a heat sink. In contrast, a lower lattice thermal conductivity is required for thermal insulation applications (e.g., thermal barrier coatings).

The formula [85] of this property is

$$K_{ph} = A \gamma_G \times \frac{M_{av} \Theta_D^3 \delta}{\gamma_G^2 n^{\frac{2}{3}} T} \quad (15)$$

where the Grüneisen parameter is γ_G , which estimates the deviation of harmonic oscillations of the phonons, where the formula is given by,

$$\gamma_G = \frac{3(1 + \nu)}{2(2 - 3\nu)} \quad (16)$$

The lower value γ_G indicates the low anharmonic characteristics in the solids. In *InPSi₃* ($\gamma_G = 1.52$) is the highest value among the three compounds in Table 6, where these materials show the lowest K_{ph} of 8.5 W/mK. The K_{ph} values of each compound are low because of the robust overlapping of acoustic and optical modes, as shown in Figure 2.

The other factor $A(\gamma_G)$ from the $eq^n - (16)$, K_{ph} , is estimated by using the Grüneisen parameters that from the following equation [86],

$$A(\gamma_G) = \frac{4.85628 \times 10^7}{2 \left(1 - \frac{0.514}{\gamma_G} + \frac{0.228}{\gamma_G^2} \right)} \quad (17)$$

The thermal conductivity is inversely proportional to temperature and reaches its lowest at high temperatures. The MTC of the studied phases has been computed by the following equation [86]:

$$K_{min} = K_B v_m \left(\frac{M}{n \rho N_A} \right)^{-\frac{2}{3}} \quad (18)$$

Materials with a lower thermal conductivity are considered suitable for thermal barrier coating (TBC) applications, with values below 1.25 (W/mK) [87]. Various materials have been explored as potential TBCs, including Ytria-stabilized zirconia (YSZ), which is the most popular TBC material, despite having a k_{min} assessment of 2.20 (W/mK) [88], $\text{RE}_2\text{T}_2\text{O}_7$ compounds, where RE represents various rare earth elements (La, Eu, Pr, Nd, Sm, Gd, Y, Er, or Lu) and T represents elements like Ti, Sn, Zr, Mo, or Pb, have k_{min} values varying from 1.40 to 3.05 W/mK [88, 89]. Furthermore, perovskite oxides and their formula ABO_3 , where A can be Sr or Ba, and B can be Ti, Zr, or Hf. These materials have minimum thermal conductivity (k_{min}) values ranging from 1.09 to 1.74 W/mK. Metal phosphates, such as ZrP_2O_7 , which has a k_{min} value of 1.15 W/mK, and HfP_2O_7 , whose k_{min} value is 0.99 W/mK [88]. The compound $\text{Mo}_4\text{Y}_2\text{Al}_3\text{B}_6$, with a k_{min} of 1.24 W/mK, is considered a potential TBC material [90]. For the titled phases, the k_{min} value is 1.8 for *AlPSi₃*, and the value decreases with substituted Ga and In in place of the Al atom.

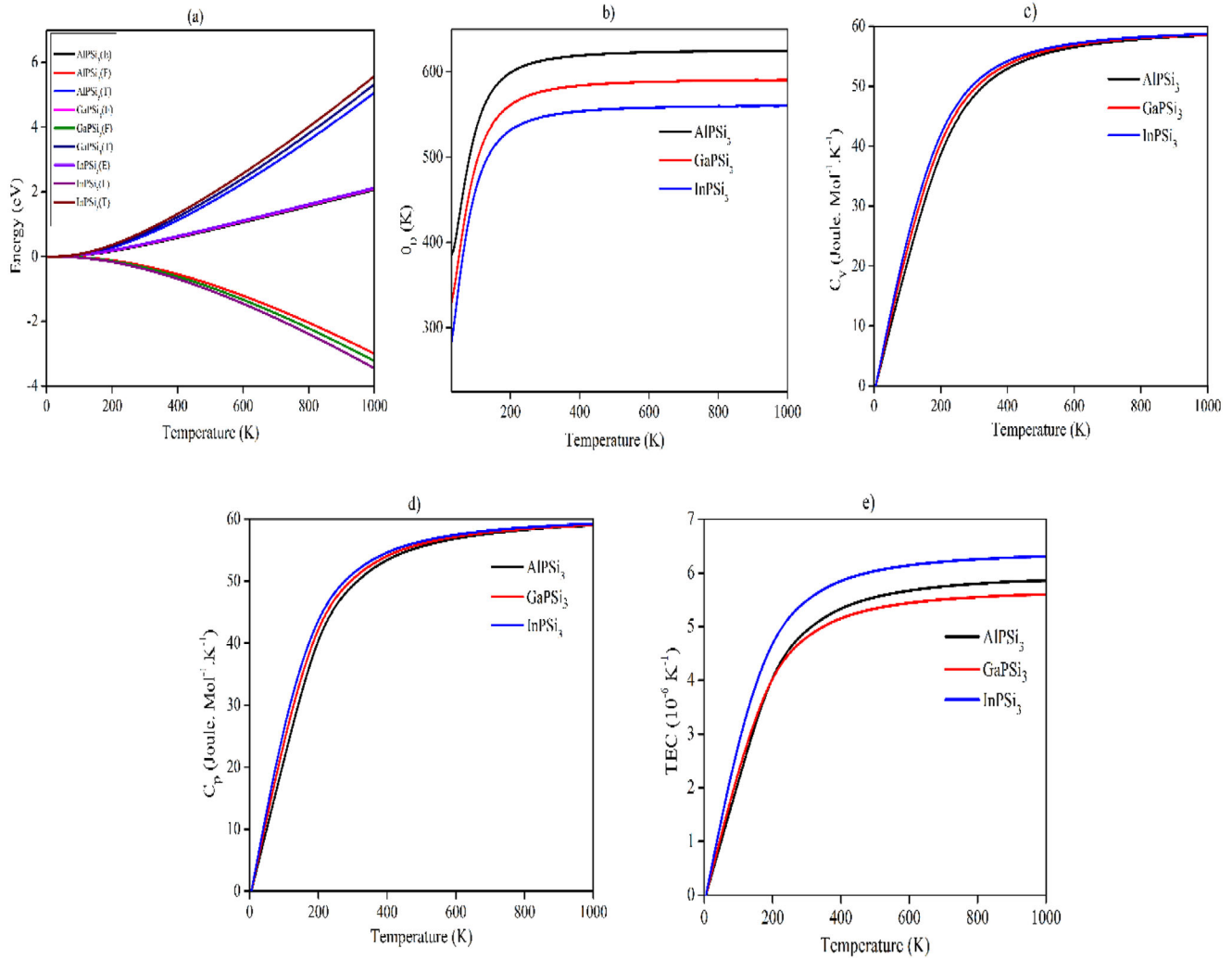


FIGURE 7 | (a) Thermodynamic functions, (b) Debye Temperature, (c) Specific heat capacity at constant volume (C_v), (d) Specific heat capacity at constant pressure (C_p), and (e) Thermal expansion coefficient.

The lowest value of $k_{\min}$ (1.02 W/mK) is obtained for InPSi₃. This compound will be suitable for possible TBC application because of its low value of $k_{\min}$, shown in Table 6. Such materials can enhance the durability and efficiency of components in aerospace, automotive, semiconductor substrates, and industrial applications.

Figure 7a presents an overview of thermodynamic potential functions, including Helmholtz free energy (F), enthalpy (E), and entropy (T.S), at zero pressure [91, 92]. Within the considered temperature range [0–1000 K], no phase transitions are observed in these thermodynamic potential functions. The values of F, E, and T.S are very nearly zero below 100 K. As temperature increases above 100 K, the free energy (F) decreases linearly, while both enthalpy (E) and entropy (T.S) increase. Enthalpy rises slightly and remains almost constant for all materials. The highest free energy (F) value is found for AlPSi₃, while the lowest is for InPSi₃. In terms of entropy (T.S), InPSi₃ displays the maximum value, while AlPSi₃ shows the lowest.

The PHDOS is used to determine the Debye Temperature (θ_D), as shown in Figure 7b. It rises with temperature, as θ_D represents

the particle's vibrational frequency, which changes with temperature. At room temperature, the Debye temperature values are: AlPSi₃ = 615 K, GaPSi₃ = 577 K, and InPSi₃ = 546 K. These values remain constant above 400 K.

Specific heat capacity defines the heat absorbed by a material for a unit of temperature increase. The values of specific heat at constant volume (C_v), obtained from thermodynamic calculations, are: AlPSi₃ = 49.17 J/mol·K, GaPSi₃ = 50.22 J/mol·K, and InPSi₃ = 51.06 J/mol·K. As shown in Figure c), C_v increases gradually with temperature up to 500 K, then remains constant above that temperature. Another measure of heat capacity is C_p , which is assessed using the formula [93]:

$$C_p = C_v (1 + \alpha \gamma_G T) \quad (19)$$

where the linear thermal expansion coefficient is α , and the Gruneisen parameter is γ_G . The α is given as follows [86]:

$$\alpha = C_v \gamma_G / 3B_T V_m \quad (20)$$

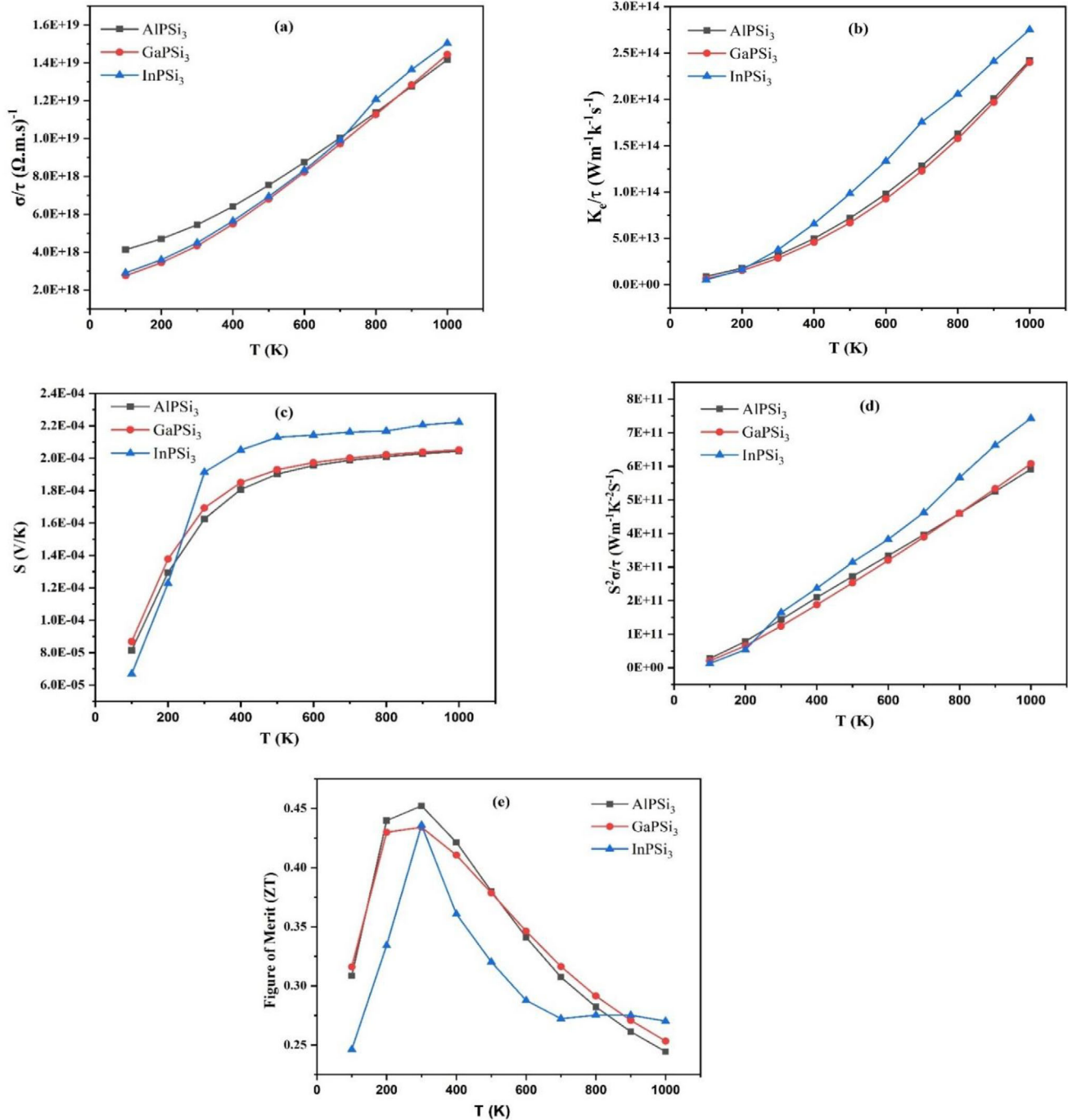


FIGURE 8 | (a) Electrical conductivity, (b) Electronic conductivity, (c) Seebeck coefficient, (d) Power factor, and (e) Thermoelectric efficiency of studied materials.

where B_T is the isothermal bulk modulus, and V_m is the molar volume.

Figure 7c,d shows the temperature-dependent values of C_v and C_p , respectively. Both values follow a similar trend, remaining constant above 500 K. The α is a function of temperature that explains the manner in which a material's length varies with temperature. At room temperature, the TEC values are: $\text{AlPSi}_3 = 4.9 \times 10^{-5} \text{ K}^{-1}$, $\text{GaPSi}_3 = 4.7 \times 10^{-5} \text{ K}^{-1}$, and $\text{InPSi}_3 = 5.5 \times 10^{-5} \text{ K}^{-1}$ displaying Figure 7e. The TEC values indicate greater resistance to thermal expansion, making them ideal for applications

requiring materials to withstand high temperatures without deformation.

3.6 | Thermoelectric Properties

In our surroundings, almost every activity or work produces heat, which we release into the environment, increasing the ambient temperature and contributing to global warming. This heat is a waste of energy and harms our environment. So, the ability to convert waste heat into electrical energy, known as

thermoelectricity, is a crucial feature. In this section, we will study the thermoelectric properties of MPSi_3 ($M = \text{Al, Ga, In}$). For this study, it is necessary to examine several transport parameters, including electrical conductivity (σ/τ), electronic thermal conductivity (K_e/τ), Seebeck coefficient (S), power factor (PF), and figure of merit (ZT). Using the BoldTrap2 code [94], we examine the transport parameters over the temperature range 100K to 1000 K, and all parameters are presented in Figure 8a–e.

Electrical conductivity $\sigma = nq\mu$, where n is the concentration of the carrier, q denotes the charge of the carrier, and μ is the mobility of the carrier, which describes how easily charge carriers move through a material [95]. Figure (a) shows a linear increase in electrical conductivity, a key feature of semiconductors, with conductivity increasing with temperature [96]. The electrical conductivity varies from $4.13\text{E}+18$ to $1.42\text{E}+19$ ($\Omega\cdot\text{m}\cdot\text{s}$)⁻¹ for AlPSi_3 , $2.75\text{E}+18$ to $1.44\text{E}+19$ ($\Omega\cdot\text{m}\cdot\text{s}$)⁻¹ for GaPSi_3 and $2.90\text{E}+18$ to $1.5\text{E}+19$ ($\Omega\cdot\text{m}\cdot\text{s}$)⁻¹ for InPSi_3 . At room temperature (300K), electrical conductivity is $5.44\text{E}+18$, $4.33\text{E}+18$, and $4.49\text{E}+18$ ($\Omega\cdot\text{m}\cdot\text{s}$)⁻¹ for AlPSi_3 , GaPSi_3 , and InPSi_3 respectively.

Electronic conductivity increases with temperature like electrical conductivity, as shown in Figure 8b. The electronic conductivity varies from $8.90\text{E}+12$ to $2.42\text{E}+14$ $\text{Wm}^{-1}\text{K}^{-1}\text{s}^{-1}$ for AlPSi_3 , $6.57\text{E}+12$ to $2.40\text{E}+14$ $\text{Wm}^{-1}\text{K}^{-1}\text{s}^{-1}$ for GaPSi_3 and $5.27\text{E}+12$ to $2.75\text{E}+14$ $\text{Wm}^{-1}\text{K}^{-1}\text{s}^{-1}$ for InPSi_3 . At room temperature (300K), electronic conductivity is $3.18\text{E}+13$, $2.86\text{E}+13$, and $3.77\text{E}+13$ $\text{Wm}^{-1}\text{K}^{-1}\text{s}^{-1}$ for AlPSi_3 , GaPSi_3 , and InPSi_3 , respectively. We observe here that electrical conductivity is a factor of 10^5 greater than electronic conductivity, which shows potential for optoelectronic applications. The total thermal conductivity is obtained from the sum of both electronic and lattice thermal conductivity [97, 98], but lattice thermal conductivity is negligible. Here, the total conductivity equals the electronic conductivity.

Another important measure is the Seebeck coefficient (S), which measures the voltage across a material. A high Seebeck coefficient is highly desirable, and a positive value indicates that holes are the predominant carriers. Figure 8c, which displays the Seebeck coefficient versus temperature, indicates that the compounds are P-type. As with electrical and electronic conductivities, compounds' Seebeck coefficients increase with temperature, but after 400 K, the values are nearly saturated. At room temperature (300 K), InPSi_3 has a higher Seebeck coefficient than the other two.

One of the most important measures is the power factor, which indicates the efficiency of a thermoelectric material in converting heat into electrical energy, and it depends on the electrical conductivity and the Seebeck coefficient, and is denoted as $\text{PF} = \sigma S^2$ [33]. Figure 8d displays that the PF also increases with increasing temperature. The power factor varies from $2.75\text{E}+10$ to $5.92\text{E} + 11$ $\text{Wm}^{-1}\text{K}^{-2}\text{s}^{-1}$ for AlPSi_3 , $2.07\text{E} + 10$ to $6.07\text{E} + 11$ $\text{Wm}^{-1}\text{K}^{-2}\text{s}^{-1}$ for GaPSi_3 and $1.3\text{E} + 10$ to $7.43\text{E} + 11$ $\text{Wm}^{-1}\text{K}^{-2}\text{s}^{-1}$ for InPSi_3 .

Another key parameter for thermoelectric materials is the figure of merit (ZT). A higher ZT indicates greater efficiency in thermoelectric materials; it is high when the power factor is high,

and the total thermal conductivity is low [99]. Figure 8e shows room-temperature (300K) ZT values of 0.45 for AlPSi_3 , 0.43 for GaPSi_3 , and 0.44 for InPSi_3 , indicating that these materials are less promising for thermoelectric applications. Beenaben et al. reported thermoelectric and optoelectronic properties of TiAgZ ($Z = \text{Al, Ga, In}$), with a ZT values of 0.30, 0.29, and 0.27 in the p-type region, and 0.23, 0.24, and 0.27 in the n-type region at 1000 K for TiAgAl , TiAgGa , and TiAgIn , respectively [32]. However, their ZT values are greater than that of some reported thermoelectric materials, such as TaPtSi ($\text{ZT} = 0.13$) [33], ReSTe ($\text{ZT} = 0.4$) [100], and LaTe ($\text{ZT} = 0.4$) [101].

4 | Conclusions

The structural, electronic, opto-electronic, thermo-mechanical, and thermoelectric properties of MPSi_3 [$M = \text{Al, Ga, In}$] have been studied. The positive elastic constants, negative formation energy, and positive phonon spectrum verify the stability of the compounds. The electronic band structure reveals that AlPSi_3 and GaPSi_3 are direct-band-gap semiconductors, whereas InPSi_3 has an indirect band gap. The E_g values are close to the well-known S.Q. limit for solar cell materials, suggesting their promise for solar cell applications. A high absorption coefficient ($>10^5$ cm^{-1}) and a low reflectivity support their potential use in solar cell technology. Low elastic moduli (B , G , Y) and Hardness parameters confirm their soft nature, while indicators (ν , G/B , CP) reveal their brittleness, and the indices predict an anisotropic nature. The $k_{\min}$ of 1.02 W/m·K for InPSi_3 suggests it could serve as a thermal barrier coating ingredient. The ZT values of 0.45 for AlPSi_3 , 0.43 for GaPSi_3 , and 0.44 for InPSi_3 at room temperature make them less promising candidates for thermoelectric applications. The direct band gap (1.5–2.0 eV) and high absorption coefficients suggest that these compounds could be suitable for top-cell absorbers in tandem solar cells.

Author Contributions

S. K. Datta: data curation, investigation, formal analysis, visualization, writing – original draft. **S. Mahmud:** formal analysis, validation, writing – review & editing. **M. M. Hossain:** formal analysis, validation, writing – review & editing. **M. M. Uddin:** validation, writing – review & editing. **M. A. Ali:** conceptualization, methodology, formal analysis, validation, project administration, writing – review & editing, supervision.

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Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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