

Exploring the electronic, elastic, optical, thermal, and structural characteristics of silicon nitride (Si₃N₄) ceramic by employing the FP-LAPW method

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Abstract:

This paper presents a comprehensive first-principles investigation into the structural, electronic, elastic, optical, thermal, and mechanical characteristics of the polymorphic ceramic β -Si₃N₄. The analysis employs the highly reliable full-potential linearized augmented plane wave (FP-LAPW) approach, executed within the robust context of density functional theory (DFT) using the WIEN2k package. Structural optimization utilizes the Perdew–Burke–Ernzerhof (PBE) version of the generalized gradient approximation (GGA). Notably, the electronic band gap is accurately determined using the superior modified Becke–Johnson (mBJ) functional, which offers enhanced predictive power over conventional approximations. The six independent elastic constants are derived directly from the stress–strain responses under minute deformations, which subsequently informs the prediction of the overall mechanical behavior of β -Si₃N₄. Band structure analysis confirms the intrinsic semiconducting nature of the compound. Optical behavior is explored by calculating the complex dielectric function $\epsilon(\omega)$ and its related parameters, including the refractive index, extinction coefficient $k(\omega)$, absorption coefficient $\alpha(\omega)$, reflectivity $R(\omega)$, and the

electron energy-loss function $L(\omega)$. Furthermore, thermal features are meticulously examined through the quasi-harmonic Debye model, enabling the determination of critical thermodynamic properties such as the equilibrium volume, bulk modulus, and specific heat capacity as a function of temperature and pressure. The computed results demonstrate excellent consistency with established theoretical and experimental data, thereby validating the methodological rigor. These findings establish the critical reliability of β -Si₃N₄ and underscore its immense potential for advanced technological and scientific applications, offering a valuable benchmark for future research in materials science.

1. Introduction

Ceramic nitrides with the general chemical formula A_3N_4 ($A = C, Si, Ge, Sn$) are well known for their outstanding physical properties, including exceptional hardness [1,2], remarkable thermal stability at high decomposition temperatures [3], and resistance to chemical attack and mechanical wear. Owing to these advantages, such materials have become indispensable in a wide range of industrial and technological applications. Among them, group-IV nitrides are of particular significance because of their broad utilization in both structural ceramics and advanced electronic devices [4]. From a crystallographic perspective, these nitrides can adopt various structural phases depending on the temperature and applied pressure conditions. Silicon nitride (Si₃N₄), composed of silicon and nitrogen atoms, exists in three distinct polymorphic modifications: α (trigonal), β (hexagonal), and γ (cubic). The α and β phases are the most stable and technologically relevant, whereas the γ phase is only obtained under extreme thermodynamic environments. The α -Si₃N₄ polymorph crystallizes in a trigonal lattice system, where each silicon atom occupies the center of a distorted tetrahedron coordinated by nitrogen atoms, forming a nearly planar configuration bonded to three Si atoms. Occasionally, oxygen atoms may substitute within this framework, giving rise to silicon oxynitride derivatives. In contrast, the β -Si₃N₄ phase exhibits a hexagonal crystal structure closely related to the α -phase, in which each Si atom is tetrahedrally bonded to four N atoms, with the nitrogen atoms located at the tetrahedral corners and Si at the center [5]. This β -modification represents the thermodynamically most stable form, typically forming at elevated temperatures [6]. The purpose of the present research is to conduct a detailed first-principles investigation of the structural, electronic, elastic, optical, and thermal characteristics of the β -Si₃N₄ ceramic, by means of the full-potential linearized amplified plane wave (FP-LAPW) approach inside the density functional theory (DFT) framework.

The remainder of this article is organized as follows: Section 2 presents the computational methodology adopted in this work, Section 3

discusses the calculated results and their implications, and Section 4 summarizes the key findings and conclusions of the study.

2. Theoretical details

The complete potential linearized enlarged plane movement (FP-LAPW) method is esteemed as one of the most precise and dependable first-principles techniques for ascertaining the ground-state characteristics of crystalline materials [7]. This method functions inside the context of density functional theory (DFT) [8,9], and in this research, it was executed using the WIEN2k computational software [10]. The generalized gradient approximation (GGA) developed by Perdew, Burke, and Ernzerhof was utilized to assess exchange–correlation effects in modeling structural properties, while the improved Becke–Johnson (mBJ) potential was applied to enhance the accuracy of electronic band-gap estimation. In the FP-LAPW formalism, the potential, charge density, and wave functions inside the unit cell are represented differently in two separate regions: inside the non-overlapping muffin-tin (MT) spheres surrounding each atom, and in the interstitial region among them. Inside the MT spheres, the wave functions are expanded using spherical harmonics, whereas in the interstitial space, a plane-wave basis set is employed. To ensure accurate convergence, the basis set size defined by the product ($RMT \times K_{max}$) was fixed at 8, where (RMT) denotes the minimum muffin-tin radius and K_{max} is the plane-wave cutoff. The wave-function expansion inside the atomic spheres was limited to an angular momentum quantum number (l_{max}) of 10, and the charge density was Fourier-expanded with a cutoff value of ($G_{max} = 14 \text{ Ryd}^{1/2}$). The muffin-tin radii for Si and N atoms were chosen as 1.46 a.u. and 1.61 a.u., correspondingly. The zone of Brillouin sampling was conducted by means of a 40 k-point mesh in the irreducible wedge to guarantee a high level of accuracy in the total-energy calculations. Finally, the $RMT \times K_{max}$ parameter and k-point mesh were carefully tested and adjusted to achieve complete energy convergence for the β -Si₃N₄ compound.

3. Results interpretation

3.1. Structural characterization

The binary nitride Si_3N_4 , which typically contains seven chemical formula units per unit cell, crystallizes in a hexagonal lattice structure assigned to the $P6_3$ space group, as shown in Figure 1. The Wyckoff atomic positions for silicon are (6h): ($x = 0.17486$, $y = 0.4064173$, $z = 0.75$), while nitrogen atoms occupy two distinct sites: (2c): ($x = 0.333333$, $y = 0.666667$, $z = 0.75$) and (6h): ($x = 0.030679$, $y = 0.329943$, $z = 0.25$). To regulate the ground-state structural limitations, the total energy (E) of $\beta\text{-Si}_3\text{N}_4$ was calculated across multiple volume configurations near equilibrium, as illustrated in Figure 2. The resulting E - V data were subsequently analyzed using Murnaghan's equation of state [13], enabling the estimation of equilibrium lattice constants and the bulk modulus. Table 1 presents a comparative summary of the calculated equilibrium parameters lattice constants (a_0 , c_0), bulk modulus (B_0), and its pressure derivative (B'_0) alongside previously reported theoretical and experimental results. The obtained data exhibit excellent agreement with published findings, reflecting the accuracy of the computational approach. Specifically, the calculated equilibrium lattice constants derived from the PBE-GGA functional show relative deviations of only 0.09% for a_0 and 0.06% for c_0 compared with experimental results [21,22]. Furthermore, the estimated bulk modulus (B_0) and its pressure derivative (B'_0), obtained via Murnaghan's equation of state, demonstrate values slightly higher than experimental observations [23], yet remain consistent with other theoretical predictions [14–18]. This minor overestimation can be attributed to intrinsic differences between exchange–correlation approximations and experimental conditions. Overall, the close match between the current results and prior literature confirms the validity of the chosen FP-LAPW–GGA computational framework for modeling $\beta\text{-Si}_3\text{N}_4$.

3.2. Elastic Properties of $\beta\text{-Si}_3\text{N}_4$

Elastic constants are essential factors that characterize a material's reaction to external stresses, offering insights into its mechanical stability, anisotropy, ductility, and hardness. This work computes the elastic characteristics of $\beta\text{-Si}_3\text{N}_4$, including bulk modulus, shear modulus, young's modulus, Poisson's ratio, anisotropy indices, hardness, and ductility criteria. The hexagonal structure of Si_3N_4 includes the autonomous elastic constants (C_{11} , C_{33} , C_{44} , C_{66} , C_{12} , and C_{13}) as a requirement for ductility. The

independent constants elastic (C_{11} , C_{33} , C_{44} , C_{66} , C_{12} , and C_{13}) for the hexagonal structure of Si_3N_4 were calculated and are shown in Table 2. Significantly, for $\beta\text{-Si}_3\text{N}_4$, these values demonstrate strong concordance with both experimental data [24] and theoretical analyses [25]. Moreover, the calculated findings comply with the Born stability criterion for hexagonal crystals [26], articulated as follows:

$$C_{44} > 0, C_{11} > |C_{12}|, (C_{11} + 2C_{12})C_{33} > 2C_{13}^2.$$

a mechanical stability confirmed by of the examined chemical.

The computed elastic coefficients provide deeper insights into the anisotropic mechanical behavior of $\beta\text{-Si}_3\text{N}_4$. Our calculations indicate that $C_{11} = C_{22} < C_{33}$, implying that the bonding strength along the [001] (c-axis) direction is stronger than along the [100] and [010] (a-b plane) directions. This result suggests that the atomic interactions in the c-axis direction contribute more significantly to the material's rigidity. The comparable values of $C_{44} = C_{55}$ and C_{66} indicate uniform shear response in different crystallographic orientations. This suggests that $\beta\text{-Si}_3\text{N}_4$ exhibits a relatively isotropic shear response, despite its hexagonal symmetry. The fact that C_{ii} ($i \leq 3$) are significantly larger than C_{ii} ($i \geq 4$) implies that $\beta\text{-Si}_3\text{N}_4$ resists unidirectional compression more effectively than shear deformation, reinforcing its structural robustness in applications requiring high compressive strength.

Elastic constants are essential for assessing different elastic characteristics, which may be calculated using the Voigt-Reuss-Hill (V-R-H) averaging technique [27–29]. In a hexagonal system, the bulk modulus (B) and shear modulus (G) are connected to the elastic constants C_{ij} as seen below:

$$B_V = (1/9)[2(C_{11} + C_{12}) + 4C_{13} + C_{33}] \quad (1)$$

$$G_V = (1/30)(M + 12C_{44} + 12C_{66}) \quad (2)$$

$$B_R = C^2/M \quad (3)$$

$$G_R = (5/2)[C^2 C_{44} C_{66}] / [3B_V C_{44} C_{66} + C^2(C_{44} + C_{66})] \quad (4)$$

$$\text{Where: } C_{66} = 1/2(C_{11} - C_{12}) \quad (5)$$

$$M = C_{11} + C_{12} + 2C_{33} - 4C_{13} \quad (6)$$

$$C^2 = (C_{11} + C_{12})C_{33} - 2C_{13}^2 \quad (7)$$

The Hill approximations for wholesale modulus (B) and shear modulus (G) are then determined as:

$$B = B_H = \frac{B_V + B_R}{2} \quad (8)$$

$$G = G_H = \frac{G_V + G_R}{2} \quad (9)$$

The poisson's ratio (ν) and young's modulus (E), which are important for discovering out how hard a material is, are provided by:

$$E = \frac{9BG}{3B+G} \quad (10)$$

$$\nu = \frac{3B-2G}{2(3B+G)} \quad (11)$$

The bulk modulus (B) derived via the Voigt–Reuss–Hill (V–R–H) averaging method is in remarkable concordance with the bulk modulus (B_0) calculated using Murnaghan's equation of state, so validating the precision and dependability of the current elastic computations. Table 3 illustrates that β -Si₃N₄ exhibits high values of bulk modulus (B), Young's modulus (E), and shear modulus (G), signifying its exceptional hardness and mechanical strength.

To evaluate brittleness and ductility, we employ the B/G ratio, a criterion introduced by Pugh [30]. According to this criterion, a critical threshold of 1.75 distinguishes between brittle and ductile materials. Compounds with $B/G < 1.75$ are brittle, while those with $B/G > 1.75$ are ductile. Our calculations yield $B/G = 1.92$, which exceeds the critical threshold of 1.75, confirming that β -Si₃N₄ is a ductile material.

Poisson's ratio (ν) and the G/B ratio serve as key indicators of a material's bonding characteristics. Covalent materials typically exhibit $\nu \approx 0.1$ and $G/B \approx 1.1$, whereas ionic materials generally show $\nu \approx 0.25$ and $G/B \approx 0.6$. In contrast, metallic materials tend to have $\nu \approx 0.33$ and $G/B \approx 0.4$ [31]. Based on our results presented in Table 3, the calculated Poisson's ratio ($\nu = 0.278$) and G/B ratio (0.52) suggest that β -Si₃N₄ exhibits ductile behavior and its bonding nature exhibits a strong ionic character.

3.3. Electronic Analysis

The band structure of the polymorph-type ceramic Si₃N₄ was computed using mBJ and PBE-GGA approximations, and the estimated values are illustrated in Figure 3. The calculations were performed along the high-symmetry directions of the Brillouin zone. As shown in the plots, the hexagonal (β) crystal structure of Si₃N₄ exhibits an indirect band gap, with the valence band maximum (VBM) occurring at Δ direction, while the conduction band minimum (CBM) is located at Γ point. This confirms that the β -Si₃N₄ phase has an indirect band gap ($\Delta_{\max} - \Gamma$), which is consistent with previous findings reported by Amy Y. et al. [32], Shang-Yuan Ren et al. [33], Yong-Nian Xu [14], and Cem Sevik et al.

[15]. A comparison study of the estimated band gap values is provided in Table 4, juxtaposing our calculated outcomes with current theoretical and data from experiments. The indirect band gap of β -Si₃N₄, calculated by the mBJ approximation, is 4.99 eV, significantly exceeding the value derived from the PBE-GGA functional. This discrepancy occurs because GGA-based functionals are known to underestimate the band gap, while mBJ offers a more precise adjustment to the exchange potential, aligning the computed values more closely with experimental findings. Table 4 indicates that the mBJ-derived band gap is more consistent with experimental data and prior theoretical predictions, hence validating the dependability of our methodology. The Density of States (DOS) analysis provides deeper insight into the electronic structure of β -Si₃N₄, illustrating the contributions of different atomic orbitals to the formation of the valence and conduction bands. Figure 4 illustrates the full density of states (TDOS) and partial density of states (PDOS) for the Si₃N₄ combination. The valence band is composed of two distinct regions:

The first region, spanning the energy range [0, -6.246 eV], arises due to the hybridization of Si-p and N-p orbitals. The second region, located within [-6.246, -12.369 eV], is primarily attributed to the hybridization between N-p and Si-s orbitals. It is noteworthy that N-s electrons do not participate in bond formation within the β -Si₃N₄ structure, as their contribution to the DOS is negligible. β -Si₃N₄ compound is characterized by a wide band gap (4.99 eV), confirming its semiconducting nature. The conduction band is formed by a mixture of s and p orbitals from both Si and N atoms, contributing to electronic transitions.

3.4. Optical properties

Understanding the optical behavior of crystalline solids is essential for unveiling their intrinsic physical characteristics, particularly constraints such as the reflectivity (R), refractive index (n), and extinction coefficient (k). These optical indicators provide valuable information regarding the electronic band structure, impurity states, and excitonic interactions, all of which play a vital role in describing the optical nature of β -Si₃N₄. Figure 5 proves a complex components real [$\epsilon_1(\omega)$] and imaginary [$\epsilon_2(\omega)$] of function the dielectric for β -Si₃N₄ under ambient pressure (0 GPa) across the 0–35 eV photon-energy range. The computed spectra reveal a clear anisotropy between the two polarization modes (xx and zz), confirming that the dielectric tensor obeys $\epsilon_{xx} = \epsilon_{yy} \neq \epsilon_{zz}$. Consequently, two distinct dielectric responses can be

distinguished, corresponding to $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$. The static dielectric constants, $\epsilon_1(0)$, are evaluated as 4.49 and 4.65 along the x- and z-axes, respectively, which are slightly higher than the values reported by Yong-Nian Xu et al. [14]. The optical transition threshold, determined from the imaginary part $\epsilon_2(\omega)$, is estimated at 4.35 eV (xx polarization) and 4.31 eV (zz polarization). These values correlate well with previous theoretical estimations (5.4–5.8 eV [14]) and agree closely with experimental data of 4.4 eV [36], 5.5 eV [37], 5.1 eV [38], and 4.55–5.3 eV [39]. Within the 0–35 eV energy window, multiple peaks appear in the $\epsilon_2(\omega)$ spectrum, indicating interband electronic transitions. The direct optical band gaps are identified as 4.17 eV for xx polarization and 4.12 eV for zz polarization. The dominant peaks in the zz component occur at 6.81 eV, 8.20 eV, and 10.62 eV, while in the xx polarization, additional peaks are observed at 6.38 eV, 7.71 eV, 9.94 eV, 10.59 eV, and 12.06 eV. The Figure 6 in (a) and 6(b) explain the spectral differences of the extinction quantity $k(\omega)$ and refractive index $n(\omega)$ for β -Si₃N₄ at zero pressure, corresponding to the xx and zz polarizations, respectively. The peak refractive index is observed at photon energies between 5.12 eV and 7.93 eV, contingent upon the polarization direction. The refractive index diminishes as photon energy increases, illustrating standard optical dispersion characteristics. The extinction coefficient $k(\omega)$ demonstrates an optical threshold (E_0) of 5.39 eV for xx polarization and 4.63 eV for zz polarization. The computed values for the static dielectric function ($\epsilon(0)$) and refractive index ($n(0)$) are presented in Table 5, indicating a modest increase relative to the values reported by Yong-Nian Xu et al. [14], while maintaining strong concordance with established theoretical studies.

Key optical parameters, including the energy loss function $L(\omega)$ and reflectivity $R(\omega)$, are related by the following equations [44, 45]:

$$R(\omega) = [k^2 + (1 - n)^2] / [(1 + n)^2 + k^2] \quad (12)$$

$$L(\omega) = \Im(\epsilon^{-1}) \quad (13)$$

The computed frequency-dependent reflectivity $R(\omega)$ for β -Si₃N₄ is depicted in Figure 7(a). The highest peaks occur within the 5–23 eV range for the xx and zz polarizations, respectively. The maximum reflectivity values reach 51% (zz polarization) and 47% (xx polarization), indicating moderate reflectivity across the UV spectrum. The static reflectivity $R(0)$ is estimated at 12% (xx polarization) and 13% (zz polarization) at $\omega = 0$, demonstrating a slight polarization dependence. The reflectivity spectrum spans the entire ultraviolet (UV) energy range, suggesting that β -Si₃N₄ is a promising candidate for optoelectronic

devices operating in UV area. Figure 7(b) illustrates the energy loss function $L(\omega)$, which elucidates plasma resonance behavior, across a range of energy 0–35 eV. The primary crests in the energy loss function are identified at 23.18 eV for zz polarization and 23.61 eV for xx polarization. The observed values align through the discoveries of Shu Xia and al. [46], who identified a maximum energy loss at approximately 24 eV. The maximum value of $L(\omega)$ correlates with a significant reduction in reflectivity $R(\omega)$, signifying the presence of plasma resonance at the plasma frequency. The spectrum $\alpha(\omega)$ of absorption for β -Si₃N₄ is illustrated at Figure 8. The absorption threshold values are computed as $\alpha_{xx} = 12.74$ eV and $\alpha_{zz} = 15.47$ eV, with absorption occurring within the 11.82–20 eV spectral range. These findings confirm the strong UV absorption capability of β -Si₃N₄, making it a suitable material for applications in UV-shielding, optoelectronic devices, and optical coatings.

3.5. Thermal properties

The thermal characteristics of β -Si₃N₄ were examined utilizing the Gibbs program [47] and the quasi-harmonic debye model. The variation of Helmholtz allowed energy with temperature and pressure was determined within the quasi-harmonic framework to characterize the thermodynamic behavior of β -Si₃N₄, facilitating a comprehensive examination of thermodynamic behavior. The Gibbs free energy function for a crystalline solid in non-equilibrium conditions, accounting for the total unit cell energy and hydrostatic PV contributions, is definite as:

$$G * (V; P; T) = A_{vib}[\theta_D(V), T] + PV + E(V) \quad (14)$$

Here A_{vib} denotes the vibrational free-energy term, evaluated under the Debye approximation by integrating over the phonon density of states [48, 49]:

$$A_{vib}(\theta_D, T) = nK_B T \left[\frac{9\theta_D}{8T} + 3 \ln \left(1 - e^{-\left(\frac{\theta_D}{T}\right)} - D\left(\frac{\theta_D}{T}\right) \right) \right] \quad (15)$$

In this context, n denotes the quantity of atoms per formula unit, while $D(\theta/T)$ signifies the Debye integral. The Debye temperature (θ_D) for an isotropic solid is defined as [49]:

$$\theta_D = \frac{\hbar}{K_B} \left[6\pi^2 V^{\frac{1}{3}} n \right]^{\frac{1}{3}} f(\sigma) \sqrt{\frac{B_s}{M}} \quad (16)$$

wherever M means the unit cell of the molecular mass, and B_s signifies the adiabatic bulk modulus, approached using static squeezability as [47]:

$$B_S \cong B(V) = V \left\{ \frac{d^2 E(V)}{dV^2} \right\} (17)$$

The function $f(\sigma)$ is defined as:

$$f(\sigma) = \left\{ 3 \left[2 \left(\frac{21+\sigma}{31-2\sigma} \right)^{\frac{3}{2}} + \left(\frac{11+\sigma}{31-\sigma} \right)^{\frac{3}{2}} \right]^{-1} \right\}^{\frac{1}{3}} (18)$$

Here σ is the ratio of Poisson, assumed to stand 0.25[50]. Under non-equilibrium conditions, $G^*(V; P; T)$ is optimized concerning V , fulfilling:

$$\left[\frac{\partial G^*(V; P; T)}{\partial V} \right]_{P, T} = 0 (19)$$

Resolving equation (16) produces the equation thermal of state (EOS), $V(P, T)$. The isothermal bulk modulus B_T , capacity heat C_V , and entropy S are supplied by [38]:

$$B_T(P, V) = V \left(\frac{\delta^2 G^*(V; P; T)}{\delta V^2} \right)_{P, T} (20)$$

$$C_V = 3nK \left[4D \left(\frac{\theta}{T} - \frac{3\theta/T}{e^{\theta/T} - 1} \right) \right] (21)$$

$$S = nk \left[4D \left(\frac{\theta}{T} \right) - 3 \ln \left(1 - e^{-\frac{\theta}{T}} \right) \right] (22)$$

Founded on the calculated E–V data over an eclectic range of pressures and temperatures, and with applying the quasi-harmonic Debye model, the thermal behavior of β -Si₃N₄ was systematically analysed. The study encompassed temperatures between 0 and 1800 K and pressures up to 8 GPa. Figure 9 illustrates the difference of equilibrium volume with temperature below different pressures. The volume expands steadily as the temperature increases, exhibiting an almost linear trend beyond 400 K. In contrast, at a fixed temperature, the

equilibrium volume reductions noticeably with rising pressure. Figure 10 shows that the bulk modulus remains nearly unchanged up to around 100 K, after which it gradually decreases with further temperature increase. At constant pressure, compressibility increases with temperature, whereas at constant temperature, it decreases when pressure is raised. The dependence of the Debye temperature (θ_D) on temperature and pressure is displayed in Figure 11. A slight reduction in θ_D occurs within the 0–100 K interval, followed by a linear decrease above 300 K. Interestingly, the variation of θ_D mirrors that of the bulk modulus under changing thermodynamic conditions. This correlation is consistent with theoretical expectations, which indicate that materials with higher hardness generally possess larger Debye temperatures, reflecting a nearly linear relationship between the two quantities. The specific heats at constant volume (C_V) and constant pressure (C_P) are also key indicators of thermal performance. Their temperature and pressure dependence is depicted in Figure 12. Both C_V and C_P rise rapidly with temperature up to about 200 K, after which the increase becomes more gradual above (300 K). C_V approaches the classical Dulong–Petit limit of $3nR = 6R = 49.98 \text{ J/mol} \cdot \text{K}$ [51]. At temperatures above 100 K, pressure exerts a stronger influence on C_P than on C_V , leading to a reduction in C_P with increasing pressure, though it does not settle to a constant value.

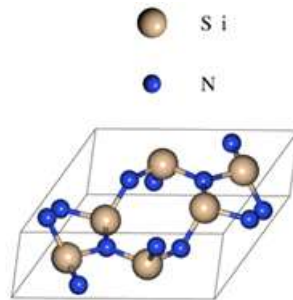


Figure 1. Crystal structure of β -Si₃N₄ showing the hexagonal unit cell.

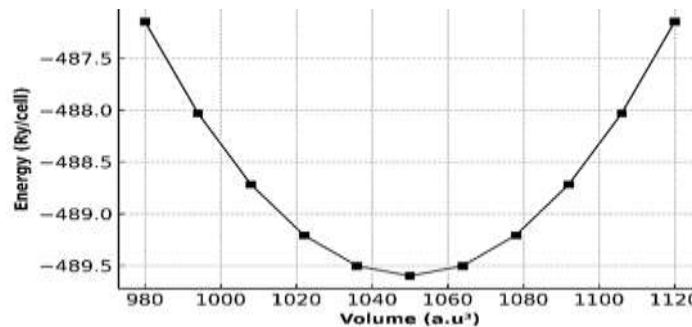


Figure 2. total energy vs volume for β -Si₃N₄.

Table 1. Comparison of the calculated equilibrium parameters (a_0 , c_0 , B_0 , and B'_0) for β - Si_3N_4 with previously reported theoretical predictions and experimental measurements.

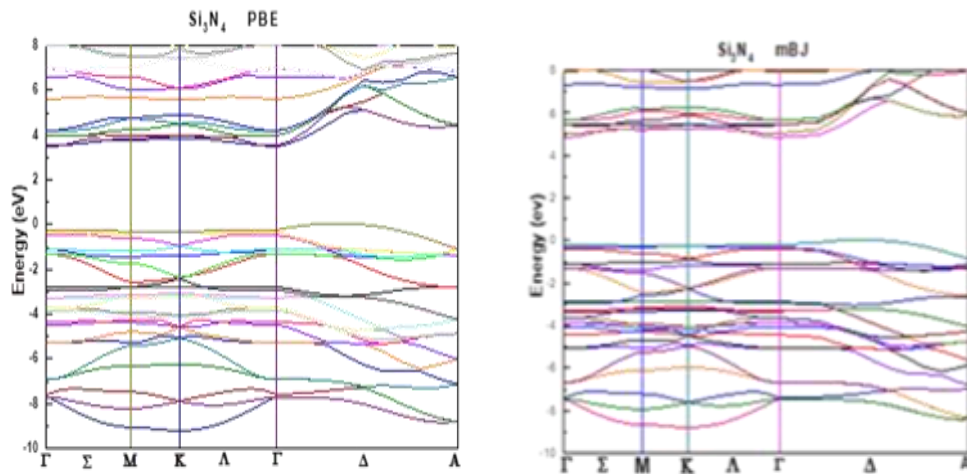
	$a_0 (\text{\AA})^\circ$	$c_0 (\text{\AA})^\circ$	$B_0 (\text{GPa})$	B'_0
Present work	7.68	2.93	248.72	4.06
Other Calculations	7.586 ^a	2.902 ^a		
	7.580 ^b	2.899 ^b		
	7.585 ^c	2.895 ^c		
	7.632 ^{d-GGA}	2.915 ^{d-GGA}		
	7.515 ^{d-LDA}	2.870 ^{d-LDA}		
	7.533 ^e	2.934 ^e	270 ^e	3.99 ^e
	7.595 ^f	2.902 ^f		
Exp	7.593 ^j	2.921 ^j		
	7.607 ^h	2.911 ^h	232.7 ^g	
	7.607 ⁱ	2.907 ⁱ		

^a[14], ^b[15], ^c[16], ^d[17], ^e[18], ^f[19], ^g[20], ^h[21], ⁱ[22], ^j[23].**Table 2.** The β - Si_3N_4 elastic constants

Structure		Elastic constants (GPa)		
		Present work	exp [24]	other calculations [25]
β - Si_3N_4	Hexagonal	$C_{11}=430.21$	$C_{11}=433$	$C_{11}=403$
		$C_{12}=151.27$	$C_{12}=195$	$C_{12}=180$
		$C_{13}=117.63$	$C_{13}=127$	$C_{13}=105$
		$C_{33}=526.72$	$C_{33}=574$	$C_{33}=526$
		$C_{44}=103.37$	$C_{44}=108$	$C_{44}=99$
		$C_{66}=123.47$	$C_{66}=119$	$C_{66}=112$

[24]^a, [25]^b**Table 3:** Elastic moduli (in GPa) of β - Si_3N_4

		B_V	B_R	B_H	G_V	G_R	G_H	B/G	E	ν
β - Si_3N_4	Present work	234.91	233.15	234.03	128.48	114.60	121.54	1.92	230.16	0.278
	Other calc.	--	--	259 ^a	--	--	--	--	--	--
		235 ^b	234 ^b	234 ^b	125 ^b	116 ^b	120 ^b	1.95 ^b	237.97 ^b	0.28 ^b

**Figure 3.** Electronic energy band structure of β - Si_3N_4 obtained at $P = 0$ GPa using PBE-GGA and mBJ approximations.

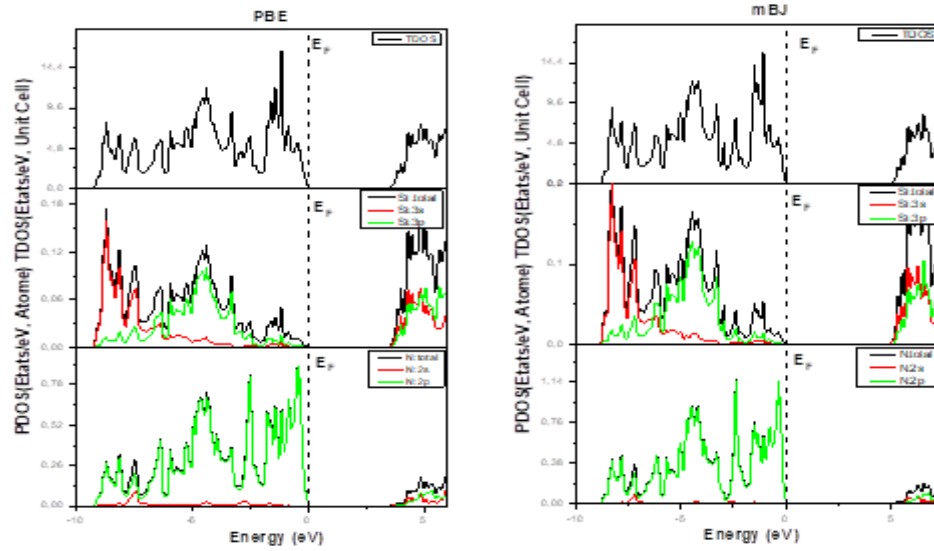


Figure 4. The computed total and partial densities of states for the β -Si₃N₄ compound using the PBE-GGA and mBJ approximations.

Table 4: Indirect energy gaps (eV) calculated for the β -Si₃N₄.

Present work		Other calculations		Exp
		PBE	mBJ	
3.44	4.99	4.2 ^a		5.3-4.7 ^e
	4.72 ^c			4.9-5.5 ^f
	4.96 ^b			5.8 ^f
		4.15 ^d		

^a[14], ^b[15], ^c[32], ^d[33], ^e[34], ^f[35].

Table 5: Determined static refractive index $n(0)$, static values of static dielectric constant $\epsilon_1(0)$, using mBJ approximation compared to other theoretical values.

β -Si ₃ N ₄	$\epsilon_{xx}(0)$	$\epsilon_{zz}(0)$	$n_{xx}(0)$	$n_{zz}(0)$	Other calculations		
	4.49	4.65	2.12	2.14	$\epsilon_{xx}(0)$	$\epsilon_{zz}(0)$	$n(\text{average})$
					4.01 ^a	3.67 ^a	1.97 ^a , 2.0 ^b , 1.99 ^c , 2.1 ^d , 2.04 ^e

^a[14], ^b[40], ^c[41], ^d[42], ^e[43]

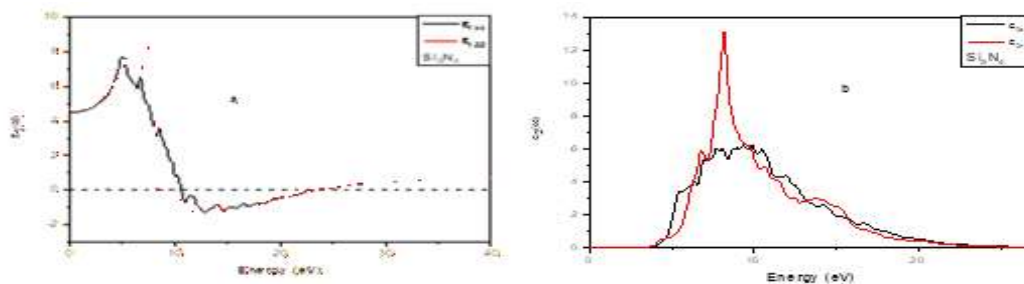


Figure 5. Complex components of the dielectric function $\epsilon(\omega)$ for β -Si₃N₄: (a) $\epsilon_1(\omega)$ and (b) $\epsilon_2(\omega)$.

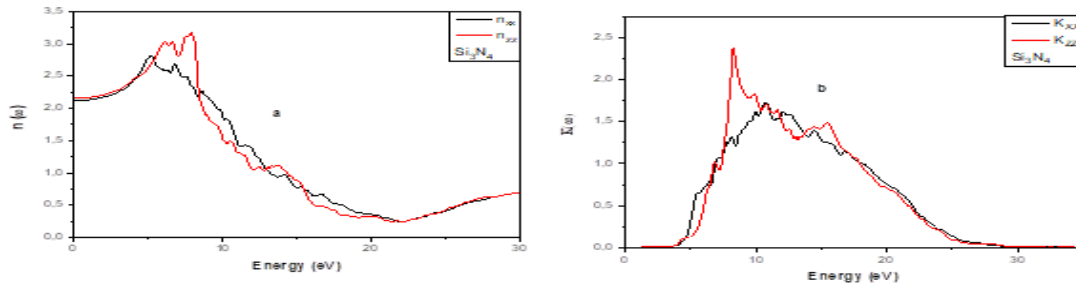


Figure 6. Calculated optical constants of β -Si₃N₄: (a) refractive index $n(\omega)$ and (b) extinction coefficient $k(\omega)$.

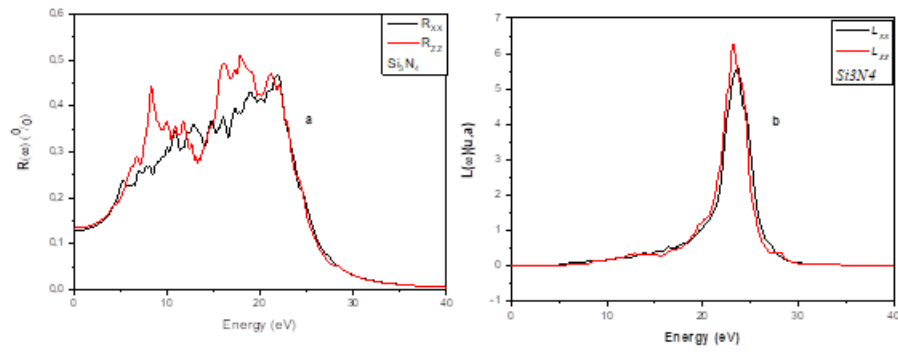


Figure 7. Frequency-dependent optical properties of β - Si_3N_4 : (a) reflectivity $R(\omega)$ and (b) energy-loss function $L(\omega)$.

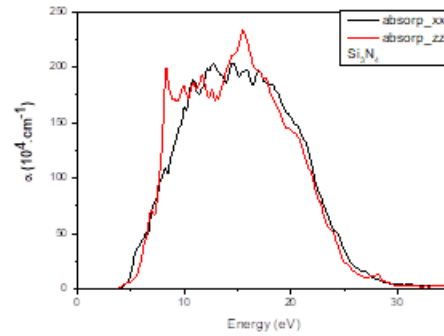


Figure 8. Variation of the absorption coefficient $\alpha(\omega)$ of β - Si_3N_4 as a function of photon energy.

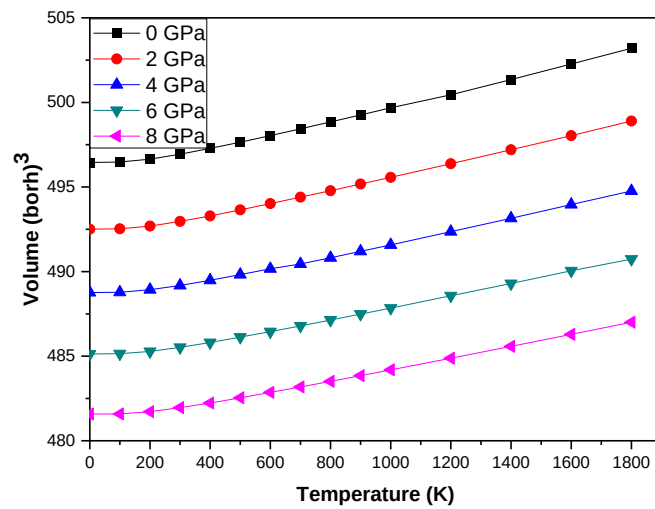


Figure 9. Temperature-dependent volume changes across various pressures for Si_3N_4

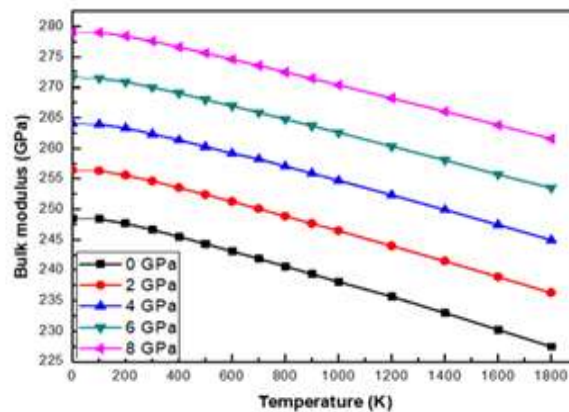


Figure 10. Temperature-dependent changes in bulk modulus across pressures various for Si_3N_4

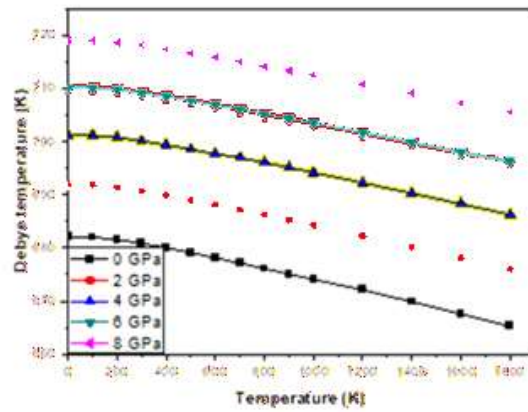


Figure 11. Variation of the Debye temperature θ_D of temperature at different pressures for β - Si_3N_4 .

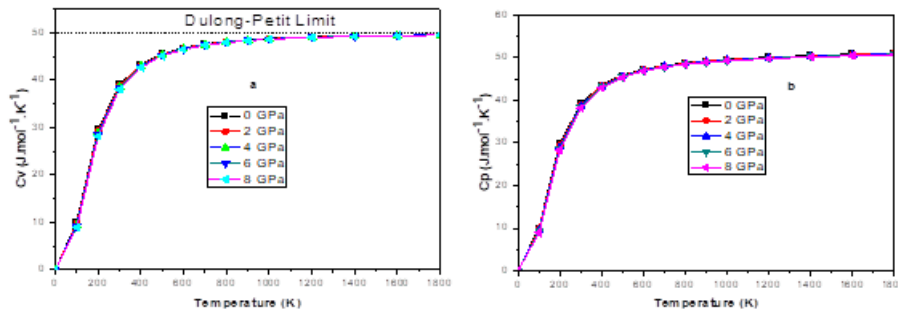


Figure 12. Variation of the heat capacities of β - Si_3N_4 with temperature at different pressures: (a) C_V and (b) C_P .

5. Conclusions

This method gives a full look at the structural, electronic, elastic, optical, and thermal characteristics of β - Si_3N_4 , utilizing the FP-LAPW method within the density functional theory (DFT) framework, with the application of the generalized gradient approximation (GGA) and the modified Becke-Johnson (mBJ) potential.

The findings indicate that β - Si_3N_4 demonstrates remarkable mechanical stability, optical anisotropy, and thermal resilience, positioning it as a viable option for high-performance applications.

The calculated ground-state parameters demonstrate strong concordance with both experimental and theoretical findings. Our results indicate that the compound is ductile, characterized by a predominantly ionic bonding nature, based on the estimates of the B/G ratio (1.92) and ν . The analysis of the electronic band structure confirms the material's classification as an indirect-bandgap semiconductor ($\Delta_{\text{max}}-\Gamma$ transition, 4.99 eV), and the examination of its optical properties indicates significant UV absorption (7–20 eV). The thermal properties indicate that β - Si_3N_4 exhibits structural stability over a broad spectrum of pressures (0–8 GPa) and temperatures (0–1800 K). The bulk modulus is stable up to 100 K, after which it gradually decreases at elevated temperatures, and the trend of the Debye temperature corresponds with theoretical predictions of hardness. The heat

capacities (C_V and C_P) demonstrate anticipated behavior, by C_V nearing the Dulong-Petit limit at elevated temperatures. The plasma resonance peak (~ 23 eV) observed in the function of energy loss ($L(\omega)$) indicates potential applications in plasmonic nanodevices. The results underscore the extensive technological applications of β - Si_3N_4 , attributed to its distinctive mechanical strength, optical properties, and thermal stability. Its high hardness, wear resistance, and chemical stability suggest extensive applications in cutting tools and high-performance ceramics

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- **Ethical approval:** The conducted research is not related to either human or animal use.
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on request from the corresponding author. The data are not publicly available due to privacy or ethical restrictions.

- **Use of AI Tools:** The author(s) declare that no generative AI or AI-assisted technologies were used in the writing process of this manuscript.

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