

Article

Hydrostatic-Pressure Modulation of Band Structure and Elastic Anisotropy in Wurtzite BN, AlN, GaN and InN: A First-Principles DFT Study

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Abstract

III-Nitride semiconductors (BN, AlN, GaN, and InN) exhibit exceptional electronic and mechanical properties that render them indispensable for high-performance optoelectronic, power, and high-frequency device applications. This study implements first-principles Density Functional Theory (DFT) calculations to elucidate the influence of hydrostatic pressure on the electronic, elastic, and mechanical properties of these materials in the wurtzite crystallographic configuration. Our computational analysis demonstrates that the bandgap energy exhibits a positive pressure coefficient for GaN, AlN, and InN, while BN manifests a negative pressure coefficient consistent with its indirect-bandgap characteristics. The elastic constants and derived mechanical properties reveal material-specific responses to applied pressure, with BN maintaining superior stiffness across the pressure range investigated, while InN exhibits the highest ductility among the studied compounds. GaN and AlN demonstrate intermediate mechanical robustness, positioning them as optimal candidates for pressure-sensitive applications. Furthermore, the observed nonlinear trends in elastic moduli under pressure reveal anisotropic mechanical responses during compression, a phenomenon critical for the rational design of strain-engineered devices. The computational results provide quantitative insights into the pressure-dependent behavior of III-N semiconductors, facilitating their strategic implementation and optimization for high-performance applications in extreme environmental conditions, including high-power electronics, deep-space exploration systems, and high-pressure optoelectronic devices.

Keywords: III-nitrides; DFT; high-pressure effect; bandgap; mechanical properties; elastic stiffness



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1. Introduction

Group III-nitride XN (i.e., X ≡ B, Ga, Al, In) semiconductors have received significant interest in recent years due to their excellent mechanical, thermal, and structural properties. These materials possess wide, direct bandgaps—except for the BN alloy, which is indirect [1] and possesses high carrier mobility [2–4], excellent thermal resistance [5,6], and exceptional

mechanical strength [7]. Such characteristics position them as some of the most promising materials for advanced optoelectronic applications, ranging from short-wavelength light-emitting diodes and high-power lasers to high-electron-mobility transistors (HEMTs) [8,9], vertical transistors, and solar cells [10].

The study of wurtzite III-nitride semiconductors under high pressure is driven by significant technological and fundamental scientific motivations. From a technological standpoint, thin films of these materials, used in devices like high-electron-mobility transistors (HEMTs) and light-emitting diodes (LEDs), are subject to substantial internal stress. This stress arises from the lattice and thermal expansion coefficient mismatches between the nitride epilayers and the underlying substrates (e.g., SiC or sapphire). This inherent strain, which possesses a hydrostatic component, can profoundly alter the electronic band structure and phonon frequencies, thereby impacting device performance, efficiency, and reliability. Consequently, understanding the effects of pressure is crucial for strain engineering and the targeted design of optoelectronic and electronic devices. Scientifically, the application of hydrostatic pressure is a powerful and clean method for tuning the interatomic distances within the crystal lattice without introducing defects. This allows for the fundamental investigation of structure–property relationships, the rigorous validation of theoretical models, and the exploration of pressure-induced structural phase transitions, which offer deep insights into the nature of interatomic bonding and the limits of material stability [11–15].

Despite their potential, enhancing the performance of III-nitride semiconductors faces various challenges, particularly under extreme conditions like high pressures or temperatures. Experimental investigations are constrained by technical limitations such as the lack of native substrates [16,17], which leads to high defect densities and lattice mismatches [18,19], as well as difficulties in achieving uniform alloy compositions in materials like InGaN and AlGaN [20,21]. Furthermore, precise control over growth techniques, such as MOCVD or MBE, is required to address issues like impurity incorporation, polarity control, and thermal-stress-induced cracking [22–24]. These challenges are compounded by high costs, time-intensive setups, and the need for advanced high-pressure growth equipment, leaving critical gaps in understanding the material properties and their behavior under extreme conditions. To overcome these hurdles, numerical methods, particularly *ab initio* approaches such as Density Functional Theory (DFT), have emerged as invaluable tools. DFT enables precise simulations of electronic, structural, and mechanical properties [25–27]. However, the optimized bandgap energy values of XN materials using Local Density Approximation (LDA) or the Generalized Gradient Approximation (GGA) functionals can frequently display significant deviations from experimental results for specific III-nitride materials. For instance, the experimental bandgap of BN is around 8.7 eV, yet Satawara reported a significantly underestimated value of 4.9 eV using the Generalized Gradient Approximation (GGA) with the PBE functional [28]. Similarly, for GaN, Gasmi reported a bandgap value of 2.044 eV [29] using the LDA functional, which significantly underestimates the experimental value of 3.4 eV [30]. In the case of InN, the experimental bandgap ranges from 0.7 eV to 1 eV [31], and the LDA-calculated value of 0.88 eV is in close alignment with this range [32]. For AlN, a bandgap value of 6.28 eV was obtained using methodologies developed by Bagayoko, Zhao, and Williams, and later refined by Ekuma and Franklin [33], which closely approximates the experimental value of approximately 6.2 eV [34]. Advancements in exchange–correlation functionals, particularly the Tran–Blaha-modified Becke–Johnson (TB-mBJ) potential, have significantly enhanced the accuracy of bandgap predictions. For example, Beldjal reported bandgap values of 0.953 eV for InN and 3.364 eV for GaN using the TB-mBJ approach [35]. These results highlight the capability of this method to closely align theoretical predictions with experimental findings, show-

casing its potential to reduce the longstanding discrepancies in semiconductor bandgap calculations. The understanding of the impact of hydrostatic pressure on the electronic and mechanical properties of nitrides and their alloys is of paramount importance. It has been reported that the bandgap energy of InN, GaN, and AlN increases with pressure, exhibiting varying pressure-dependent rates, which significantly influence the performance of optoelectronic devices [36]. E. Güler's study demonstrated that AlN maintains its ionic bonding structure even at pressures as high as 50 GPa [37]. In contrast, Hangbo Qin et al. conducted a comparative study on the effects of pressure on GaN, focusing on both wurtzite and cubic crystal structures [38]. III-Nitride (III-N) materials—boron nitride (BN), aluminum nitride (AlN), gallium nitride (GaN), and indium nitride (InN)—are widely recognized for their exceptional electronic, optical, and mechanical properties. Their high thermal conductivity, wide bandgap tunability, and structural robustness make them essential for next-generation optoelectronic, power, and high-frequency devices. Additionally, their wurtzite crystal structure exhibits a strong polar nature along the [0001] c-axis, leading to spontaneous and piezoelectric polarization effects that significantly influence their electronic and mechanical behavior under external stimuli, such as pressure. The literature research on the effects of hydrostatic pressure underscores the critical role of this parameter in the understanding and optimization of nitride semiconductors for a wide range of applications. Therefore, this study employs first-principles DFT calculations to systematically investigate the electronic, elastic, and mechanical properties of wurtzite-structured III-N materials under varying pressure conditions. By providing detailed numerical insights, this research aims to bridge the gap between theoretical predictions and experimental advancements, ultimately contributing to the development of more efficient and resilient semiconductor technologies under precise pressure conditions.

2. Computational Method

III-Nitrides exhibits a wurtzite hexagonal and cubic structure under ambient conditions [39]; the hexagonal wurtzite structure is defined by the lattice parameters $a = b \neq c$, $\alpha = \beta = 90^\circ$, and $\gamma = 120^\circ$, belonging to the space group $P6_3mc$. Figure 1 illustrates the conventional unit cell and the supercell ($2 \times 2 \times 2$) of the XN wurtzite structure.

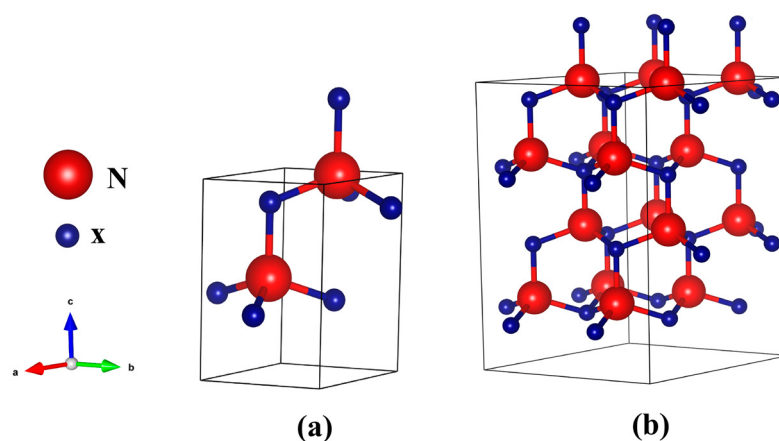


Figure 1. Structural representation of hexagonal wurtzite XN: (a) unit cell, (b) the supercell ($2 \times 2 \times 2$).

Studying the effect of pressure on various properties of wurtzite XN materials, geometry optimization was first performed using multiple methods implemented in the CASTEP program [40]: Local Density Approximation (LDA), Generalized Gradient Approximation (GGA), and Local Density Approximation with Hubbard U correction LDA+U [41]. Meanwhile, the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm [42] and Vanderbilt ultra-soft pseudopotentials [43] were used to optimize the crystal models except for InN,

where norm-conserving pseudopotential was applied. The electronic wave function cut-off energy was set at 800 eV for all materials. As for Brillouin-zone integration, Monkhorst–Pack grids of $9 \times 9 \times 9$ for BN and AlN and $10 \times 10 \times 10$ for GaN and InN were employed. The convergence tolerance of the energy, maximum force, maximum displacement, and maximum stress were set at 10^{-5} eV/atom, 0.03 eV/Å, 0.001 Å, and 0.05 GPa, respectively. To ensure the accuracy of the calculated bandgap energy, the Hubbard correction was applied to the valence electrons using the parameters listed in Table 1 below. Furthermore, the optimized bandgap energy and their pressure dependencies for XN wurtzite materials were calculated using the previously mentioned exchange–correlation potentials. In the second part of this study, the pressure effect on the mechanical properties bulk modulus B, shear modulus G, Poisson’s ratio ν , and Young’s modulus E and the elastic stiffness constants C_{ij} were computed as a function of pressure within the LDA framework. Subsequently, the Voigt–Reuss–Hill approximation [44] was employed to accurately derive the effective mechanical properties, providing a comprehensive understanding of the pressure-induced variations in the structural stability of these materials.

Table 1. Electronic configuration and Hubbard energy correction parameters for the valence electrons of each element.

		Electronic Configuration	Energy (eV)
InN	In	[Kr]4d ¹⁰ 5s ² 5p ¹	-
	N	1s ² 2s ² 2p ³	-
BN	B	1s ² 2s ² 2p ¹	12
	N	1s ² 2s ² 2p ³	12.75
GaN	Ga	[Ar]3d ¹⁰ 4s ² 4p ¹	3.75
	N	1s ² 2s ² 2p ³	3.5
AlN	Al	[Ne]3s ² 3p ¹	3.5
	N	1s ² 2s ² 2p ³	4.25

The LDA+U approach was chosen to correct for the self-interaction error inherent in standard LDA or GGA functionals, which often underestimate the bandgap. This is particularly relevant for the interaction between localized valence electrons (e.g., N-2p and B-2p in BN) and for materials like GaN, where shallow semicore d-electrons hybridize with the N-2p valence band. This method enhances the accuracy of bandgap predictions without the high computational cost of hybrid functionals and has been effectively used in systems without open d or f shells [45,46]. The U values in Table 1 were determined empirically through systematic calculations. For each material, the U value for the cation semicore state (e.g., Ga-3d) was fixed based on the literature, while the U value for the N-2p orbitals was varied incrementally. The final U parameters selected were those that produced a calculated bandgap in closest agreement with established experimental values.

3. Results and Discussion

3.1. Bandgap Energy and Structural Parameters of XN Materials

To validate our numerical results, we initiated the study by conducting geometry optimizations for wurtzite XN structures employing various exchange–correlation potentials. The calculated lattice parameters and the unit cell volume V_0 without a pressure effect are compared with corresponding numerical and experimental values; to quantify the precision of our calculated lattice parameters, we computed the relative errors in a and c, denoted as $\Delta a(\%)$ and $\Delta c(\%)$, respectively. A detailed comparison is presented in Table 2.

Table 2. Optimized lattice constants of wurtzite XN using different exchange–correlation energy.

Structure	Methods	a(Å)	$\Delta a(\%)$	c(Å)	$\Delta c(\%)$	$V_0(\text{Å}^3)$	Ref.
BN	LDA	2.52	1.29	4.17	1.07	23.03	This study
	LDA	2.50	2.07	4.169	1.09	-	[47]
	LDA+U	2.46	7.71	4.07	7.66	21.39	This study
	GGA	2.5527	0.011	4.2215	0.15	23.82	This study
	Experimental	2.553	-	4.215	-	-	[48]
GaN	LDA	3.1554	1.06	5.1453	0.76	44.36	This study
	LDA	3.156	1.05	5.145	0.77	44.373	[49]
	LDA+U	3.1249	2.02	5.0836	1.95	42.99	This study
	GGA	3.2245	1.10	5.2521	1.29	47.29	This study
	GGA	3.242	1.65	5.28	1.83	48.075	[49]
	Experimental	3.1893	-	5.1851	-	-	[50]
AlN	LDA	3.0637	1.48	4.9011	1.58	39.84	This study
	LDA	3.084	0.83	4.948	0.64	-	[51]
	LDA+U	3.0012	3.50	4.7655	4.30	36.66	This study
	GGA	3.1249	0.48	5.0089	0.58	42.35	This study
	GGA	3.12	0.32	5.00	0.40	-	[52]
	Experimental	3.11	-	4.98	-	-	[53]
InN	LDA	3.529	0.25	5.70	0.05	61.53	This study
	LDA	3.544	0.42	5.762	1.03	-	[54]
	LDA+U	3.30	6.47	5.30	7.06	50.26	This study
	GGA	3.608	2.23	5.833	2.27	65.79	This study
	GGA	3.614	2.40	5.883	3.15	-	[54]
	Experimental	3.538	-	5.703	-	-	[55]

Hence, for each compound, the first relative error reported corresponds to the *a* lattice parameter and the second to the *c* lattice parameter; for BN, GGA provides the closest agreement with experiment, showing minimal deviations of just 0.011% and 0.15%. LDA slightly underestimates the lattice parameters with relative errors of 1.29% and 1.07%, while LDA+U results in the largest underestimations, reaching 3.64% and 3.44%. For GaN, GGA yields modest deviations of 1.10% and 1.29%, indicating reasonable predictive capability. LDA+U performs less accurately with errors of 2.02% and 1.95%. In contrast, LDA achieves the best accuracy, with relative deviations of only 0.11% and 0.03%. In the case of AlN, GGA again performs well, with relative errors of 0.48% and 0.58%. LDA underestimates both parameters slightly more, with deviations of 1.48% and 1.59%. LDA+U shows the poorest agreement, introducing larger discrepancies of 3.50% and 4.31%. For InN, LDA offers excellent accuracy, with minimal deviations of 0.25% and 0.05%. GGA, however, overestimates both parameters, yielding relative errors of 1.98% and 2.28%. Consequently, GGA provides better agreement for BN and AlN, as it enhances the description of electron–electron interactions in systems with mixed covalent and ionic bonding. In contrast, LDA delivers the most accurate results for InN, showing its suitability for materials with strong ionic character and minimal long-range interactions. These results demonstrate that the choice of exchange–correlation scheme significantly influences predictive accuracy and should be carefully matched to the material’s bonding and electronic structure.

Table 3 summarizes the calculated bandgap energies of the investigated wurtzite XN materials using various exchange–correlation functionals in the absence of hydrostatic pressure. Our optimized bandgap values show good agreement with both theoretical and experimental references, particularly when employing the GGA and LDA+U schemes. For AlN and GaN, the LDA+U approach yields direct bandgap energies of 6.176 eV and 3.36 eV, respectively, which are in close concordance with the corresponding experimental

values of 6.2 eV [34] for AlN and 3.4 eV for GaN [30]. This highlights the effectiveness of the Hubbard correction for materials with wide bandgaps. In the case of InN, the GGA functional yields a bandgap of 0.976 eV, a value well-positioned inside the experimental range of 0.7–1.0 eV [31], confirming that GGA offers a good estimate for this material. As expected, all these materials exhibit direct bandgaps, except for BN, which has an indirect bandgap. For BN, the LDA+U scheme predicts a bandgap of 6.846 eV, which shows excellent agreement with the theoretical value of 6.86 eV [1]. Nevertheless, this result remains substantially lower than the experimentally observed direct bandgap of 8.7 eV [56]. Thus, the LDA+U approach demonstrates superior accuracy in predicting the bandgap of wide-bandgap semiconductors such as GaN, AlN, and BN. Conversely, for narrow-bandgap materials like InN, the conventional GGA and LDA functionals exhibit better agreement with experimental data, making them more appropriate for such systems. The band structures corresponding to the calculated bandgap energies, which closely align with the experimental values as discussed in Table 3, are presented in Figure 2.

Table 3. Bandgap energies of wurtzite XN compounds calculated using different exchange–correlation functionals, in the absence of hydrostatic pressure.

Structure	Methods	Bandgap Energy (eV)	Ref.
BN	LDA	4.914	This study
	GGA	5.204	This study
	LDA+U	6.846	This study
	experimental	8.7 ± 0.5	[56]
GaN	LDA	2.088	This study
	GGA	1.671	This study
	LDA+U	3.36	This study
	experimental	3.4	[30]
AlN	LDA	4.659	This study
	GGA	4.11	This study
	LDA+U	6.176	This study
	experimental	6.2	[34]
InN	LDA	1.057	This study
	GGA	0.976	This study
	experimental	0.7–1.0	[31]

Figure 3 illustrates the optimized bandgap energies of wurtzite XN materials across pressures ranging from 0 to 40 GPa, demonstrating pressure-induced variations in their electronic properties. The findings reveal distinct material-specific behaviors, with consistent patterns observed for GaN, BN, and InN regardless of the computational method used. For BN (Figure 3a), the bandgap energy decreases with increasing pressure, starting at 6.846 eV at 0 GPa and dropping to 6.635 eV at 40 GPa under the LDA+U scheme, showing a decreasing rate of $-0.005275 \pm 9.7 \times 10^{-5}$ eV/GPa; a comparable pressure-induced reduction in bandgap was also observed by Silvetti et al. [57], supporting the consistency of this trend. This reduction, observed across all schemes, is due to the material's indirect-bandgap nature. However, for GaN (Figure 3b), the bandgap increases nonlinearly with a quadratic variation, rising from 3.36 eV at 0 GPa to 4.05 eV at 40 GPa, regardless of the exchange–correlation approximation (LDA, GGA, or LDA+U). In contrast, AlN (Figure 3c) demonstrates a unique behavior depending on the exchange–correlation scheme. The LDA+U approximation predicts mostly an independent behavior under pressure effect, with a near-zero slope (~ 0.00128 eV/GPa). Moreover, for the LDA functional, the bandgap energy exhibits a linear increase at low pressures (up to 10 GPa) with a rate of 0.0315 eV/GPa. Beyond this threshold, the bandgap stabilizes, indicating a saturation

region where further pressure increases have minimal effect. However, the GGA functional shows a similar trend, where the linear regime extends up to 30 GPa, with a slightly higher rate of 0.033 eV/GPa. Beyond this critical point, the bandgap also reaches a saturation phase. This trend demonstrates that while the general trend of bandgap energy variation with pressure is consistent for most materials across computational methods, AlN demonstrates significant sensitivity to the choice of exchange–correlation approximations, emphasizing the critical role of theoretical models in predicting these types of electronic properties of semiconductors under pressure.

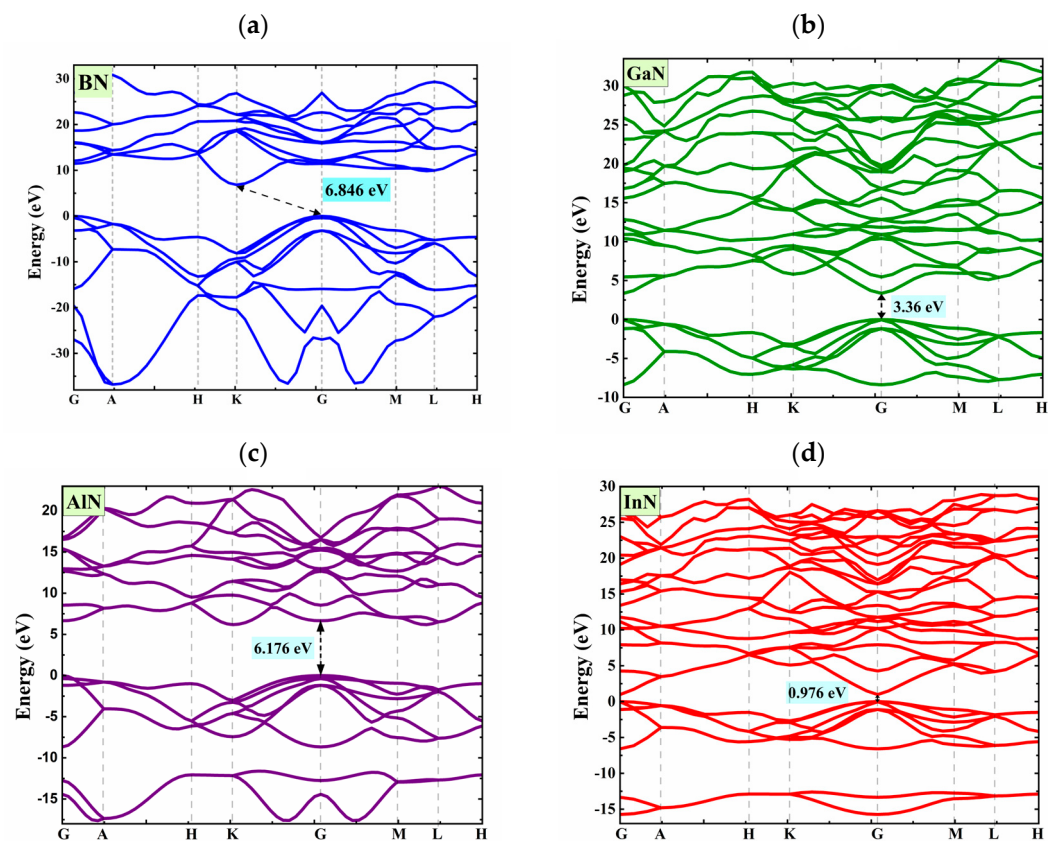


Figure 2. Electronic band structures of wurtzite III-nitrides calculated: (a) BN, (b) GaN, (c) AlN, (d) InN.

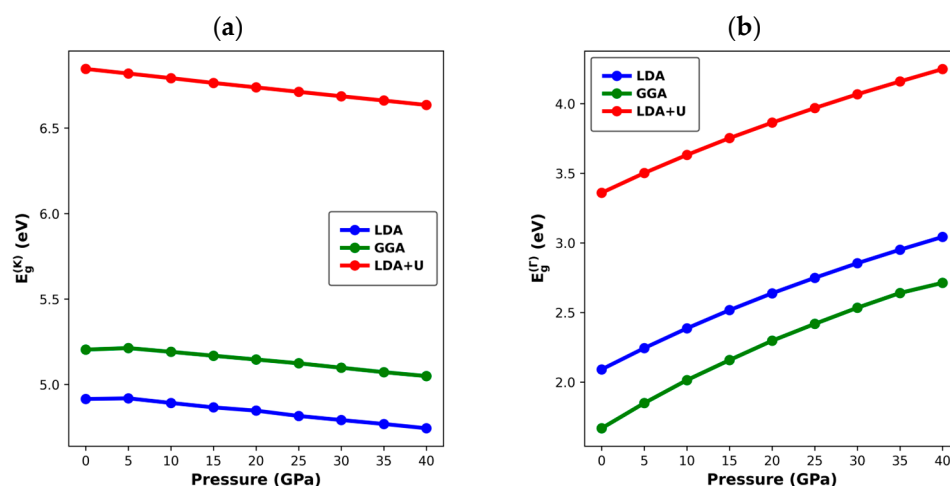


Figure 3. Cont.

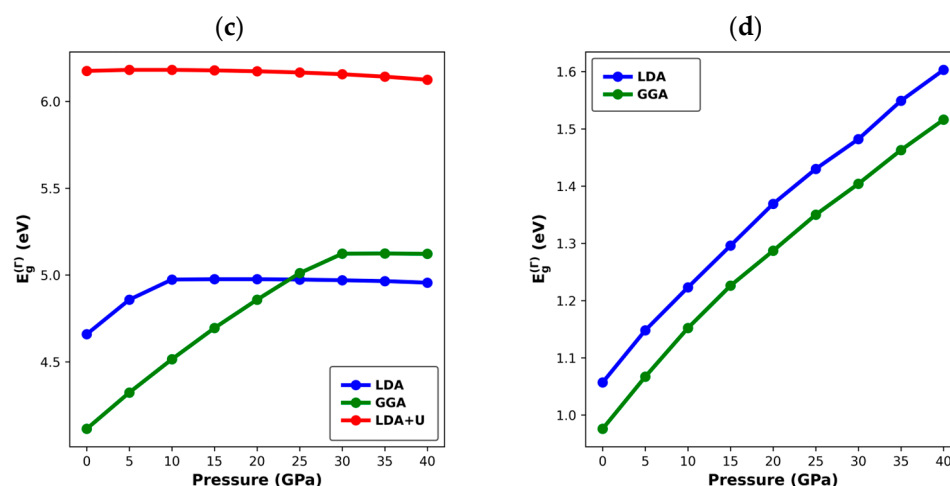


Figure 3. Pressure dependence of bandgap energy in wurtzite III-nitrides calculated using different DFT approaches (LDA, GGA, and LDA+U): (a) BN, (b) AlN, (c) GaN, and (d) InN.

In addition, InN (Figure 3d) exhibits a consistent increase in bandgap energy, from 0.976 eV at 0 GPa to 1.509 eV at 40 GPa under the GGA approximation, showing its high sensitivity to pressure. Notably, the pressure-induced increase in bandgap energy observed for these direct-bandgap III-nitride materials is in excellent agreement with prior theoretical and experimental investigations, thereby reinforcing the robustness and credibility of our computational predictions [58,59].

3.2. Elastic Constants of XN Materials

The elastic stiffness constants C_{ij} describe how a material responds to stress and its impact on a material's crystal structure and morphology deformation. These constants are important for understanding the mechanical properties of materials, especially their resistance to deformation. In hexagonal crystal structures, there are five independent elastic stiffness constants: C_{11} , C_{12} , C_{13} , C_{33} and C_{44} . The Born stability criteria are indicated [60] by the following:

$$\begin{pmatrix} C_{11} > 0 \\ (C_{11} - C_{12}) > 0 \\ C_{44} > 0 \\ (C_{11} + C_{12})C_{33} > 2C_{13}^2 \end{pmatrix} \quad (1)$$

Here, LDA approximation is used to describe the exchange–correlation potential and the elastic stiffness constants of wurtzite XN semiconductors without hydrostatic pressure as is summarized in Table 4 alongside experimental and theoretical data for comparison. For BN, C_{11} (976.95 GPa) and C_{33} (1071.48 GPa) closely match theoretical values (i.e., 982 GPa and 1077 GPa), demonstrating its exceptional rigidity and resistance to axial deformation. Similarly, the shear constant C_{66} (424.05 GPa) is in perfect agreement with the reference value, affirming the strong lattice cohesion in BN. But, for GaN, the calculated C_{11} (370.48 GPa) and C_{33} (416.39 GPa) are close to the experimental ranges (390 ± 15 GPa and 398 ± 20 GPa), indicating high resistance to compression along the x and z axes, and moderate deviations for C_{12} and C_{13} suggest anisotropic coupling between lattice directions, while C_{44} and C_{66} validate its ability to resist shear deformation. However, AlN exhibits stiffness constants C_{11} (410.53 GPa) and C_{33} (400.99 GPa) that agree well with experimental values (401.2 ± 0.5 GPa and 368.9 ± 27 GPa), demonstrating reliable mechanical behavior. The shear constants C_{44} (121.96 GPa) and C_{66} (121.96 GPa) also align closely with experimental data, confirming the ability of the computational model to capture AlN's shear response accurately. Moreover, InN, the most flexible of the materials studied, has

the lowest stiffness constants, with a C_{11} value of 227.5 GPa closely matching the experimental range of 225 ± 7 GPa, accurately reflecting InN's axial rigidity. The C_{33} constant (241.42 GPa) slightly underestimates the experimental value of 265 ± 3 GPa, which may be due to weak interlayer interactions or limitations in the computational modeling. However, the shear constants C_{44} (48.47 GPa) and C_{66} (54.84 GPa) align well with experimental values (55 ± 3 GPa and theoretical expectations, respectively), while C_{13} (81.38 GPa) deviates more significantly, compared to 108 ± 8 GPa.

Table 4. Calculated elastic constants (GPa) of wurtzite XN semiconductors at ambient pressure (0 GPa) using the LDA approach: comparison between present calculations and literature values.

Structure	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	Ref.
BN	976.95	128.85	53.88	1071.48	346.43	424.05	This study
	982	134	74	1077	388	424	[61]
GaN	370.48	129.76	90.64	416.39	97.5	120.36	This study
	374.35	126.56	80.85	441.94	98.86	123.89	[49]
	390 ± 15	145 ± 20	106 ± 20	398 ± 20	105 ± 10	123 ± 10	[62]
AlN	403.34	138	104.56	372.19	120.46	132.67	This study
	398	142	112	383	127	128	[63]
	401.2 ± 0.5	135 ± 0.5	96.3 ± 22.1	368.9 ± 27	122.6 ± 0.2	—	[64]
InN	227.5	118.06	95.85	241.42	48.47	54.84	This study
	223	115	92	224	48	—	[65]
	225 ± 7	109 ± 8	108 ± 8	265 ± 3	55 ± 3	—	[66]

The elastic stiffness constants of wurtzite BN, presented in the Figure 4a, exhibit a monotonic increase with rising pressure, demonstrating a strong linear correlation with the applied pressure. The constant C_{11} increases linearly from 976.95 GPa at 0 GPa to 1209.51 GPa at 40 GPa, with a rate of 5.576 ± 0.07 GPa/GPa, while C_{33} follows a similar trend, rising from 1071.48 GPa at 0 GPa to 1369.7 GPa at 40 GPa, with a rate of 7.483 ± 0.125 GPa/GPa. The other rigidity constants exhibit a more moderate increase, with C_{12} , C_{13} , C_{44} and C_{66} increasing at rates of 2.659 ± 0.018 , 1.582 ± 0.02 , 0.954 ± 0.026 and 1.551 ± 0.04 GPa/GPa, respectively. This consistent linear behavior confirms that BN is highly resistant to applied pressure, maintaining its structural integrity and mechanical stability. These characteristics make BN an excellent candidate for applications requiring exceptional hardness and thermal stability [67,68]. However, the elastic stiffness constants of GaN display a more complex behavior compared to BN, as shown in Figure 4b. Moreover, the longitudinal stiffness constants C_{11} and C_{33} increase at rates of 3.72 ± 0.07 GPa/GPa and 4.39 ± 0.1 GPa/GPa, respectively, with C_{33} showing slight nonlinearity at higher pressures. The off-diagonal components C_{12} and C_{13} rise more significantly, at 4.18 ± 0.07 GPa/GPa and 3.93 ± 0.07 GPa/GPa, respectively, highlighting enhanced lattice coupling and increasing resistance to lateral deformations. In contrast, the shear moduli C_{44} and C_{66} decrease at rates of -0.19 ± 0.02 GPa/GPa and -0.23 ± 0.02 GPa/GPa, respectively, indicating a reduction in shear resistance and an increased tendency for plastic deformation or structural adjustments at elevated pressures. This contrasting behavior suggests that while GaN retains overall mechanical robustness, its ability to resist shape deformation diminishes under extreme compression, which could have implications for its high-pressure performance in optoelectronic and structural applications. The elastic strength constants of wurtzite AlN, presented in Figure 4c, exhibit distinct pressure-dependent trends, encompassing both linear and nonlinear variations.

The longitudinal resistance constant C_{11} increases linearly from 403.34 GPa at 0 GPa to 542.7 GPa at 40 GPa, with a rate of 3.466 ± 0.054 GPa/GPa, indicating a consistent enhancement in resistance to axial deformation. Similarly, C_{12} and C_{13} exhibit a steady linear increase, reaching 303.15 GPa by a rate of 4.116 ± 0.006 GPa/GPa and 253.37 GPa by a rate of 3.710 ± 0.01 GPa/GPa, respectively, at 40 GPa, reflecting a strengthening of interatomic interactions under compression. In contrast, the axial stiffness constant C_{33} follows a linear trend up to approximately 25 GPa, beyond which it exhibits nonlinear behavior, suggesting the onset of saturation effects or structural modifications within the hexagonal lattice. Significant deviations are also observed in the shear moduli: while C_{44} exhibits a moderate yet linear increase from 120.46 GPa to 131.97 GPa, a rate of 0.287 ± 0.004 GPa/GPa, C_{66} undergoes a slight but nonlinear reduction from 132.67 GPa to 119.77 GPa with increasing pressure. This decrease in C_{66} suggests a pressure-induced weakening in shear resistance, potentially attributable to anisotropic lattice distortions. For InN, shown in Figure 4d, we demonstrate the linear and nonlinear behaviors of its elastic constants under pressure. C_{11} (3.04 ± 0.07 GPa/GPa), C_{12} (5.03 ± 0.03 GPa/GPa), and C_{13} (4.75 ± 0.03 GPa/GPa) increase linearly, indicating progressive stiffening, while C_{33} (2.54 ± 0.11 GPa/GPa) shows a nonlinear trend with a slower increase at higher pressures, indicating anisotropic effects. The shear moduli C_{44} (-0.56 ± 0.01 GPa/GPa) and C_{66} (-1 ± 0.03 GPa/GPa) decrease, implying a weakening of shear resistance and potential structural instability.

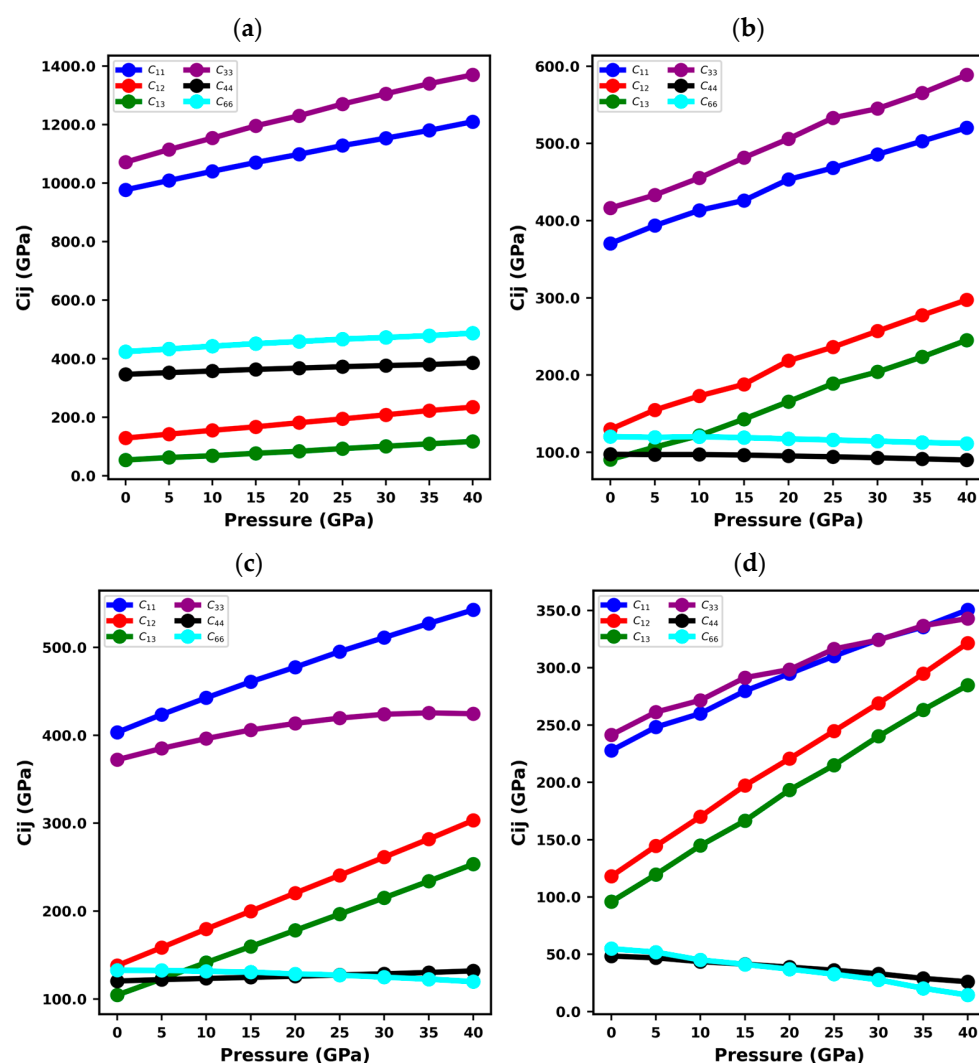


Figure 4. Pressure dependence of elastic stiffness constants (C_{ij}) for wurtzite III-nitrides: (a) BN, (b) GaN, (c) AlN, (d) InN.

3.3. Mechanical Properties of XN Materials

The bulk modulus B is a fundamental parameter that quantifies a material's resistance to compression. It is defined as the ratio of an infinitesimal increase in pressure to the corresponding relative volume change. This modulus provides insight into the incompressibility of a material, with higher values indicating greater resistance to volume reduction under applied pressure. Within the Voigt–Reuss approximation [44], B can be accurately predicted using the calculated elastic constants:

$$B_V = \frac{1}{9}[C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] \quad (2)$$

$$B_V = \frac{1}{9}[C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] \quad (3)$$

$$B_R = [S_{11} + S_{22} + S_{33} + 2(S_{12} + S_{13} + S_{23})]^{-1} \quad (4)$$

Here, B_V and B_R denote the upper and lower bounds of the bulk moduli of the polycrystalline aggregate, respectively. The elastic compliance S_{ij} is provided by the following:

$$S_{ij} = \frac{1}{C_{ij}} \quad (5)$$

The shear modulus of polycrystals can be expressed by the following equations:

$$G_V = \frac{1}{15}[(C_{11} + C_{22} + C_{33}) - (C_{12} + C_{13} + C_{23}) + 3(C_{44} + C_{55} + C_{66})] \quad (6)$$

$$G_R = 15[4(S_{11} + S_{22} + S_{33}) - 4(S_{12} + S_{13} + S_{23}) + 3(S_{44} + S_{55} + S_{66})]^{-1} \quad (7)$$

where G_V and G_R are the upper and lower bounds of shear moduli, respectively. Then, the effective bulk and shear moduli, B and G , can be predicted according to the Voigt–Reuss–Hill approximation:

$$B = (B_V + B_R)/2 \quad (8)$$

$$G = (G_V + G_R)/2 \quad (9)$$

Additionally, the elastic modulus E and the Poisson's ratio ν of polycrystalline can be provided by formulas:

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

$$\nu = \frac{3B - 2G}{6B + 2G} \quad (11)$$

The mechanical properties of wurtzite BN, GaN, AlN, and InN were calculated at 0 GPa and summarized in Table 5 below:

Table 5. Calculated mechanical properties of wurtzite XN semiconductors at ambient pressure (0 GPa): comparison between present calculations and the literature values.

Structure	B (GPa)	G (GPa)	E (GPa)	ν	Ref.
BN	388.72	405.17	902.09	0.113	This study
	397 [69]	410 $\pm$ 30 [69]	860 $\pm$ 40 [69]	0.12 [70]	-
GaN	197.705	117.47	294.15	0.252	This study
	195 [71]	161 [72]	295 [73]	0.23 $\pm$ 0.06 [74]	-
AlN	207.59	129.8	322.24	0.241	This study
	207.9 $\pm$ 6.2 [75]	132.8 [75]	308 [76]	0.245 [77]	-
InN	146.25	55.49	148.65	0.33	This study
	152 $\pm$ 5 [66]	43 [71]	149 $\pm$ 5 [78]	0.359 [79]	-

BN exhibited the highest values for bulk modulus ($B = 388.72$ GPa), shear modulus ($G = 405.17$ GPa), and Young's modulus (i.e., $E = 902.09$ GPa), significantly surpassing the other materials. This exceptional stiffness arises from the strong covalent B–N bonds, attributed to the short bond length of $1.45 \text{ \AA}$ [80], combined with a high degree of ionicity due to the substantial electronegativity difference between boron and nitrogen. These factors contribute to BN's remarkable resistance to deformation. Furthermore, BN's low Poisson's ratio ($\nu = 0.113$) indicates minimal lateral expansion under axial stress, reinforcing its brittle nature. In addition, for GaN and AlN, the presence of strong but slightly less ionic bonds compared to BN results in moderate mechanical properties. AlN, with a slightly higher electronegativity difference between Al and N compared to Ga and N [81], exhibits slightly greater values of B (207.59 GPa vs. 197.705 GPa), G (129.8 GPa vs. 117.47 GPa), and E (322.24 GPa vs. 294.15 GPa). This difference highlights the stronger bonding and lattice rigidity in AlN relative to GaN. Both materials show moderate Poisson's ratios ($\nu = 0.241$ for AlN and $\nu = 0.252$ for GaN), indicating a balanced combination of rigidity and ductility. InN, possessing the weakest bonding among the group-III nitrides, exhibits the lowest mechanical strength due to its long bond length and relatively low electronegativity difference between indium and nitrogen. The combination of the large ionic radius of indium and the extended In–N bond length ($2.14 \text{ \AA}$) results in significantly reduced bond stiffness [80]. Consequently, InN demonstrates the lowest values for bulk modulus ($B = 146.25$ GPa), shear modulus ($G = 55.49$ GPa), and Young's modulus (i.e., $E = 148.65$ GPa), indicating high compressibility and low resistance to deformation. Meanwhile, its high Poisson's ratio ($\nu = 0.33$) reflects substantial lateral expansion under uniaxial stress, highlighting its increased ductility. This behavior stems from the weaker atomic interactions and greater structural flexibility within the InN lattice, distinguishing it from its more rigid BN, AlN, and GaN counterparts.

Figure 5 illustrates the influence of hydrostatic pressure, ranging from 0 to 40 GPa, on the mechanical properties of XN nitrides. The investigated properties include the bulk modulus, shear modulus, Young's modulus, and Poisson's ratio. It is observed that the bulk modulus of the four studied materials (Figure 5a) exhibits a linear increase with increasing pressure. The corresponding rates of variation are 3.40 ± 0.02 , 3.38 ± 0.03 , 3.99 ± 0.05 , and 4.14 ± 0.04 for BN, AlN, GaN and InN, respectively. In contrast, the shear modulus (Figure 5b) displays a distinct behavior depending on the material. While for BN, it increases linearly with a rate of 1.49 ± 0.03 , a linear decrease is observed for AlN, GaN, and InN, with respective decline rates of -0.17 ± 0.03 , -0.11 ± 0.02 and -0.83 ± 0.03 . Regarding Young's modulus (Figure 5c), its behavior as a function of pressure appears similar to that of the shear modulus. Specifically, it follows a linear increase for BN, with a variation rate of 1.49 ± 0.03 , while it decreases linearly for AlN, GaN, and InN, with respective decline rates of -0.17 ± 0.03 , -0.11 ± 0.02 and -0.83 ± 0.03 . The behavior of Poisson's ratio (Figure 5d) differs significantly from that of the other elastic moduli. For BN, it follows a linear trend with a variation rate of $1.12 \times 10^{-3} \pm 2.27 \times 10^{-5}$. In contrast, for AlN, GaN and InN, its increase under pressure exhibits a quadratic trend, indicating a more pronounced nonlinear response of these materials to hydrostatic compression.

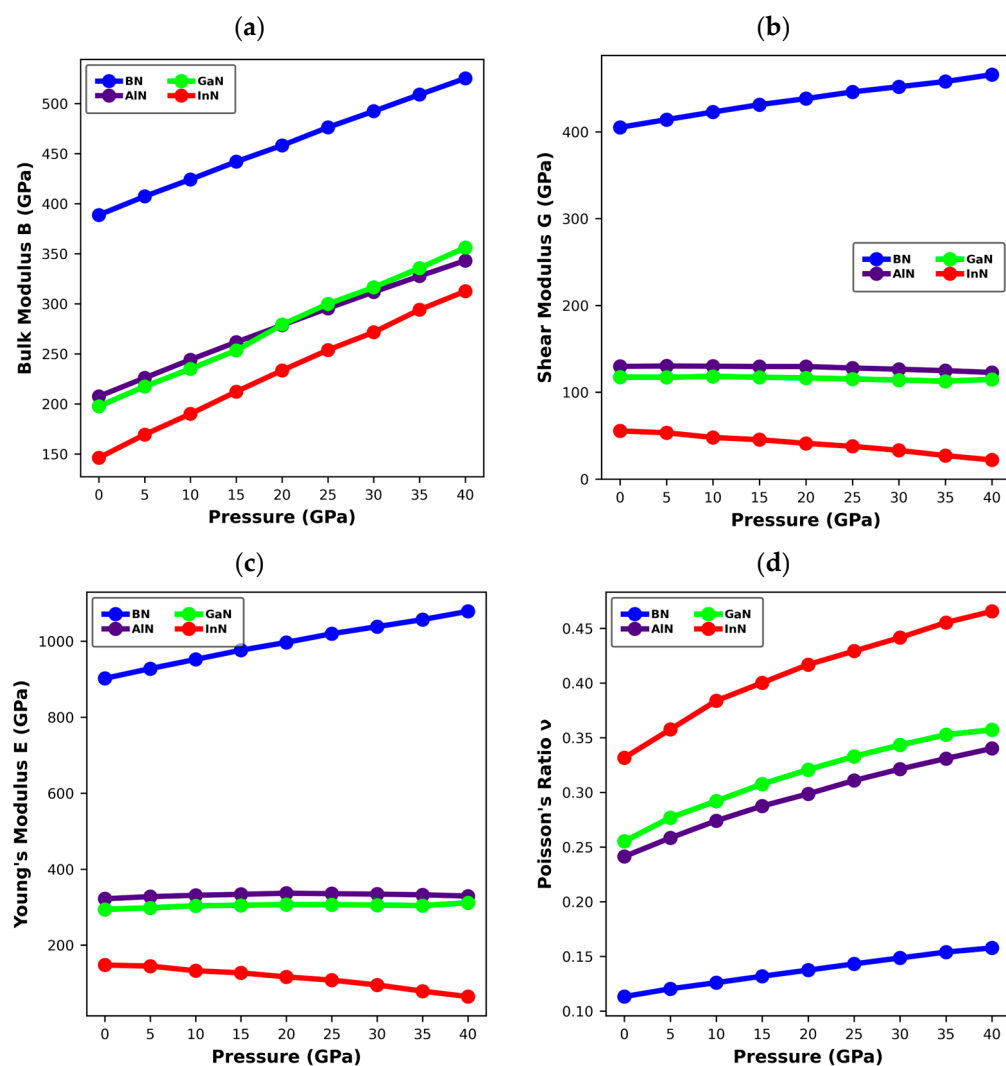


Figure 5. Pressure dependence of mechanical properties for wurtzite III-nitrides from 0 to 40 GPa: (a) bulk modulus B, (b) shear modulus G, (c) Young's modulus E, and (d) Poisson's ratio ν .

4. Conclusions

This study employed first-principles Density Functional Theory calculations to systematically characterize the hydrostatic pressure-induced modulations in electronic and mechanical properties of wurtzite III-N semiconductors (BN, AlN, GaN and InN). The computational analysis yielded several significant findings with fundamental and applied implications. The bandgap evolution under pressure exhibits material-specific behavior, with GaN, AlN, and InN demonstrating systematic bandgap expansion with increasing pressure, whereas BN manifests a contrasting trend of bandgap reduction attributable to its indirect-bandgap nature. Notably, the LDA+U formalism provided superior accuracy in bandgap estimations compared to alternative exchange–correlation functionals. Mechanical characterization revealed distinctive material-dependent responses, with BN exhibiting exceptional rigidity and resistance to deformation under pressure, while InN demonstrated superior ductility among the examined semiconductors. GaN and AlN displayed intermediate stiffness properties, rendering them particularly suitable for high-power electronic applications where thermal and mechanical resilience are requisite. Analysis of elastic constants revealed pronounced anisotropic elastic responses, particularly in GaN and InN, which exhibit nonlinear pressure-dependence in their elastic behavior. This anisotropy has significant implications for strain-engineered semiconductor devices, where directional mechanical properties critically influence performance metrics. The computational re-

sults demonstrate robust consistency with established experimental measurements and theoretical benchmarks, substantiating the validity of the methodological approach. The implementation of multiple exchange–correlation functionals provided comprehensive perspective on the electronic and mechanical behavior of III-N materials under pressure conditions. These findings constitute valuable quantitative data for the design optimization of high-pressure electronic and optoelectronic devices. Future research directions may profitably explore temperature-dependent effects, defect engineering strategies, and experimental validation studies to further refine predictive models for III-N semiconductor behavior under extreme environmental conditions.

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