Advanced Physical Research
Vol.6, No.3, 2024, pp.225-238
https://doi.org/10.62476/apr63225

# A THEORETICAL STUDY OF THE PHYSICAL PROPERTIES OF HEXAGONAL GALLIUM NITRATE USING DENSITY FUNCTIONAL THEORY

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**Abstract.** First-principles calculations based on density functional theory (DFT) have been used to investigate structural, electronic, optical and thermodynamic aspects of the α-GaN crystal. Based on local density approximations (LDA), Generalized gradient approximation (GGA) and meta-generalized gradient approximation (m-GGA) functional methods, the band gap energies of α-GaN crystals have been estimated as 1.962 eV, 2.069 eV and 2.354 eV. The band gap energies that are presented in these studies are in accordance with the ones from the other experimental and theoretical studies. Besides, our findings give us knowledge about the electronic and optical properties of α-GaN crystal. The band gap energies in the α-GaN crystal are the key factors that define its electrical and optical characteristics. They are the energy range in which the electrons can be exited from the valence band to the conduction band, which in turn affects the material's conductivity and the ability of the material to absorb and emit light. The approximate of our results with the previous researches indicates the reliability of our findings and thus increases our knowledge of α-GaN's electronic and optical phenomena. The orbital characteristics of the Ga and N atoms were found by simulating the density of state and the partial density of state for α-GaN. Besides the analysis of the band structure, density of states and optical properties of the compound we also included. The results show that α-GaN has a direct bandgap, which is at the G point in the Brillouin zone. This is the reason for its great potential for the development of optoelectronic devices. Also, we use the three approximations that are given earlier to find the optical characteristics (the absorption coefficient) of the compound. In addition to that, the thermodynamic properties that can be calculated like Debye temperature, enthalpy, free energy, entropy and heat capacity enable us to understand the thermal behavior of the compound better. The heat capacity of α-GaN is detected to be 17.3 $Jmole^{-1}K^{-1}$, with a Debye temperature of 824.6K. This research will offer a detailed interpretation of α- G-N, covering all its basic properties and the possible applications in optoelectronic and electronic devices. The results of this study are very important and the new technologies that will be developed based on the α-GaN research will be very beneficial.

***Keywords:*** *α-GaN, structural, electronic, optical properties, thermodynamic properties.*

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***Received:*** *28 August 2024;* ***Accepted:*** *1 October 2024;* ***Published:*** *16 October 2024.*

## 1. Introduction

The development of devices for near-ultraviolet optoelectronic becomes more viable by using gallium nitride (GaN). GaN has a direct band gap around 3.4 eV which is highly valuable for such technologies' providing ample prospects for optoelectronic

**How to cite (APA):**
Noori, A.F., Ghaleb, A.M. & Salih, A.I. (2024). A theoretical study of the physical properties of hexagonal gallium nitrate using density functional theory. *Advanced Physical Research*, *6*(3), 225-238 https://doi.org/10.62476/apr63225

advancements (Vaudo *et al*., 1996). It is critical to understand the optical property of this material because it's capable to form solid solutions with InN and AlN. This feature grants it high resistance to radiation and allows the making of electroluminescent devices that can emits colors from orange all the way to ultraviolet. In order to disclose properties of this material, we may examine its optical properties in certain directions. Here the interest is justified twice: firstly, optical properties are one such value that can be linked directly to the material's properties themselves and secondly, this way it is possible to determine the corresponding value for our goal – to realize the potential of the material in diverse applications. Some studies of the optical properties of hexagonal GaN have been conducted. To date, the vast majority of them are uninformative, since it has been studied in a narrow region of the scatters and most of them are visible luminescence and photo reflectance, which are there only to help determine the fundamental Bandgap (Kawashima *et al*., 1997; Logothetidis *et al*., 1995; Lambrecht *et al*., 1995). As a result of various experiments, it has been found that w-GaN at room temperature is a direct-gap semiconductor. The measured value of this Band gap is 3.26 (Kauer & Rabenau, 1957), 3.39 (Maruska & Tietjen, 1969) and 3.41 (Powell *et al*., 1993) eV. It is also known that, at room temperature and pressure, the wurtzite structure is the thermodynamically stable form of w-GaN. The electronic characteristics of wurtzite-type gallium nitride (w-GaN) have been calculated in numerous studies; however, there are discernible discrepancies between experimental and theoretical values, especially in the band gap case. Furthermore, different computations have produced differing conclusions about the band gap of w-GaN. Several calculations have utilized ab initio LDA to estimate the band gaps for w-GaN. Reported values range from 1.9188 eV to 2.31 eV (Nunez-Gonzalez *et al*., 2008; Bahmed & Aomar, 2010; Abu-Jafar *et al*., 2000; Rubio *et al*., 1993; Wright & Nelson, 1994); the second value is 0.74 eV lower than the experimentally recorded minimum. The researchers used an empirical pseudopotential method to study the electronic properties of wurtzite-type group III nitride compound semiconductors, GaN, InN and AlN (Rezaei *et al*., 2006). Theoretical band gaps for the quasiparticle energies can be obtained through different calculations involving the Green's function (G) and the dressed Coulomb (W) approximation (GW). These calculations allow us to determine the energy gaps in a theoretical framework (Rubio *et al*., 1993; Wright & Nelson, 1994; Rezaei *et al*., 2006; Kaczkowski, 2012). The values obtained from the experiment, which are 3.4 eV, are quite similar to the values mentioned in the text (Magnuson *et al*., 2010). It is worth noting that the GW calculation goes beyond the scope of the ground-state theory, DFT. It is evident from the aforementioned theoretical results that additional work is required, especially in the context of ab initio DFT calculations. The thermodynamic analysis of GaN deposition has been explored in several recent papers. These studies rely on reliable thermodynamic data to ensure accurate results. It is crucial to use trustworthy data when conducting such calculations. Thermodynamic information for solid GaN can be found in tables (Knacke *et al*., 1991) and has been recently evaluated (Przhevalskii *et al*., 1998; Moustakas *et al*., 1999). Regrettably, the data displays significant dispersion, indicating the necessity for further research. Many researches have been conducted using the density function theory and within the LDA, GGA and U+LDA approximations (Shihatha *et al*., 2022; Ghaleb *et al*., 2024; Ghaleb & Ahmed, 2022). Using DFT-based first-principles calculations, the structural, electronic, optical and thermodynamic properties of wurtzite and GaN have been examined in this work.

## 2. Computational Method

With the implementation of the LDA, GGA and m-GGA approaches, the CASTEP program (Segall *et al*., 2002) has become an indispensable resource for accurate DFT calculations, providing reliable and comprehensive data. The utilization of the Perdew-Burke-Ernzerhof exchange-correlation in these techniques is crucial. GaN adopts a hexagonal wurtzite configuration with space group P63mc when at room temperature. This structure is defined by lattice constants where a equals b, c and lattice angles α equals β equals 90° and γ equals 120° (Li & Ouyang, 2005) show in Figure 1.

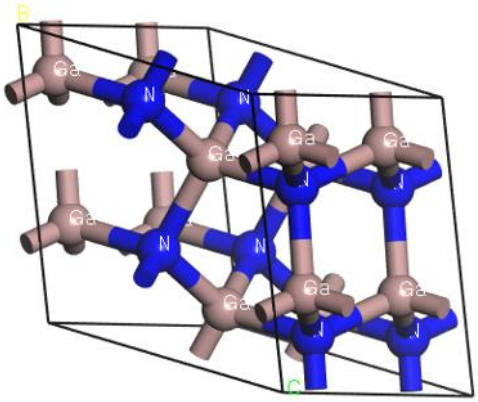



**Figure 1.** The crystal structure of α-GaN the conventional hexagonal cell

Every computation was done in a 5×5×2 grid. We have thoroughly studied the convergence tests of the total energy for the k-point sampling and plane wave energy cut off. LDA, GGA and m-GGA functions were executed via energy cutoffs: 1115eV, 880eV and 880eV, respectively. After the run, the final set of energies has been obtained. The energy-cutoff for the local density approximation (LDA) and generalized gradient approximation (GGA) in thermodynamic calculations are 590eV and 1061eV; but in order to achieve greater accuracy, they are better adjusted to 1061eV for the meta-GGA approximation. The forming is done by changing 5 × 5 × 2 k-point into the already approximately well-chosen mesh of the Brillouin zone obtained using the Monkhorst-Pack scheme (1976; 1977) the set of parameters can be defined and utilized to fulfill the sustainability of total energy of the DFT calculation such as ionic positions by the conjugate gradient method, lattice parameters and volume relaxation of the cell. Therefore, keeping the force and stress utilized as inputs in the system will provide a precise and reliable ground to predict the system's behavior down to the atomic level. Identification of important parameters such as convergence of required $2\times10^{-5}$eV per atom for the results of DFT calculations to draw meaningful conclusions and help in understanding complex systems is vital. The relaxation searches of all the atoms are monitored by saturated distributed forces throughout the optimization process. When the forces acting on all points appear to be less than the specified threshold value, the optimization procedure is finished. In this case, the interactions with the neighbors' organic atoms were found to be less than 0. 01 eV/Å. The force of interaction between atoms is limited to 0.03eV/nm, the crystal stress convergence criterion is set at 0.05GPa and the maximum displacement of atoms is restricted to 0.001nm, resulting in the optimization process being halted. The self-consistent field achieves convergence with an accuracy of $1\times10^{-6}$eV. Identify the valence electron configuration of the atom by choosing

Ga and N, with configurations of $3d^{10}4s^{2}4p^{1}$ and $2s^{2}2p^{3}$, respectively. Upon meeting the convergence criteria mentioned above, it signifies that the crystal has attained a structurally stable state. The optimized unit cell model was used to calculate the energy band structure and density of states, as well as the optical and thermodynamic properties.

## 3. Results and Discussion

### *3.1. Structural properties*

(P63/mc, No186) is the space group associated with the hexagonal wurtzite structure of gallium nitride. One Ga atom donates three electrons to one N atom during the formation of GaN, forming the ions Ga(+3) and N(-3). A covalent bond and the compound GaN are created when N and Ga share these electrons in Table 1, we have documented the computed lattice parameters and equilibrium volumes in their ground state using each approximation exchange-correlation (LDA, GGA and m-GGA). Additionally, we have included the findings from prior research on wurtzite GaN crystals for reference and comparison purposes. The results of the calculations demonstrate a high level of agreement with previous theoretical (Yoshikawa *et al*., 2004) and experimental data (Qin *et al*., 2014), effectively highlighting the validity and reliability of the study's calculations and as a result, it is utilized to compute the phase transition and energy band gap in more detail. We observe from our data that the lattice constant approximations in Qin et al. (2014) were in agreement with the practical results, but not with the theoretical results, with the percentage of difference ranging from 3 percent (LDA) to 5 percent (GGA). On the other hand, the volume unit cell of the GGA approximation showed the best agreement with the experimental data.

**Table 1.** The lattice parameters for α-GaN in the wurtzite phase were compared between the calculated and experimental values. The calculated values were determined using different approximations such as LDA, GGA and m-GGA

| Phase | Approach | $\mathbf{a}_\circ = \mathbf{b}_\circ(\text{Å})$ | $\boldsymbol{c}_\circ(\text{Å})$ | $V(\text{Å})$ | Reference |
|---|---|---|---|---|---|
| **α-GaN** | LDA | 3.189 | 5.185 | 45.137 | present work |
| | GGA | 3.189 | 5.185 | 45.665 | |
| | m-GGA | 3.189 | 5.185 | 45.443 | |
| | LDA | 3.156 | 5.145 | 44.373 | Monkhorst & Pack, (1976). |
| | GGA | 3.242 | 5.28 | 48.075 | Monkhorst & Pack, (1976). |
| | Experiment | 3.189 | 5.185 | 45.671 | Janotti et al. (2006) |

### *3.2. Electronic structure*

The Castep software is used to generate the k-points along high symmetry and follow the k-path in order to ascertain the band structure. Figure 2(a, b, c) shows the energy band structure of bulk GaN. The difference in electrical properties between metals, semiconductors and insulators can be ascertained through the energy gap between their occupied and unoccupied energy levels. Under the Fermi level is the valence band and above the Fermi level is the conduction band. The difference in energies for the conduction band minimum and valence band maximum has been computed as the band gap. Figure 2(a, b, c) displays the calculated band gap diagram for the α-GaN phase using LDA, GGA and m-GGA methods. Figure 2(a) shows that LDA's band diagram lacks a clear gap at the G point, indicating its metallic nature. Although the band diagram in

Figure 2(b) shows a gap that can be seen using the GGA method, suggesting that the compound is a semiconductor, this method does not yield the correct band gap as determined experimentally. Because of this, band gap estimates from the LDA and GGA methods are lower; for this reason, electronic calculations employ the m-GGA method is used for electronic calculation. The band diagram, shown in Figure 2(c) utilizing the m-GGA method, demonstrates that the conduction band's minimum and the valence band's maximum are situated in a line at the G point. As a result, a direct band gap of 3.5eV in α-GaN is observed, which is in accordance with the experimental data (Janotti *et al*., 2006). After performing the calculations through the approximations we mentioned above and comparing our results with the theoretical (Wright & Nelson, 1994; Magnuson *et al*., 2010) and experimental results (Janotti *et al*., 2006), we notice that the m-GGA approach gives a good match to the experimental data, as shown in Table 2. The calculation outcome indicates that GaN possesses a direct band gap, rendering it a compelling material for applications in optoelectronics.

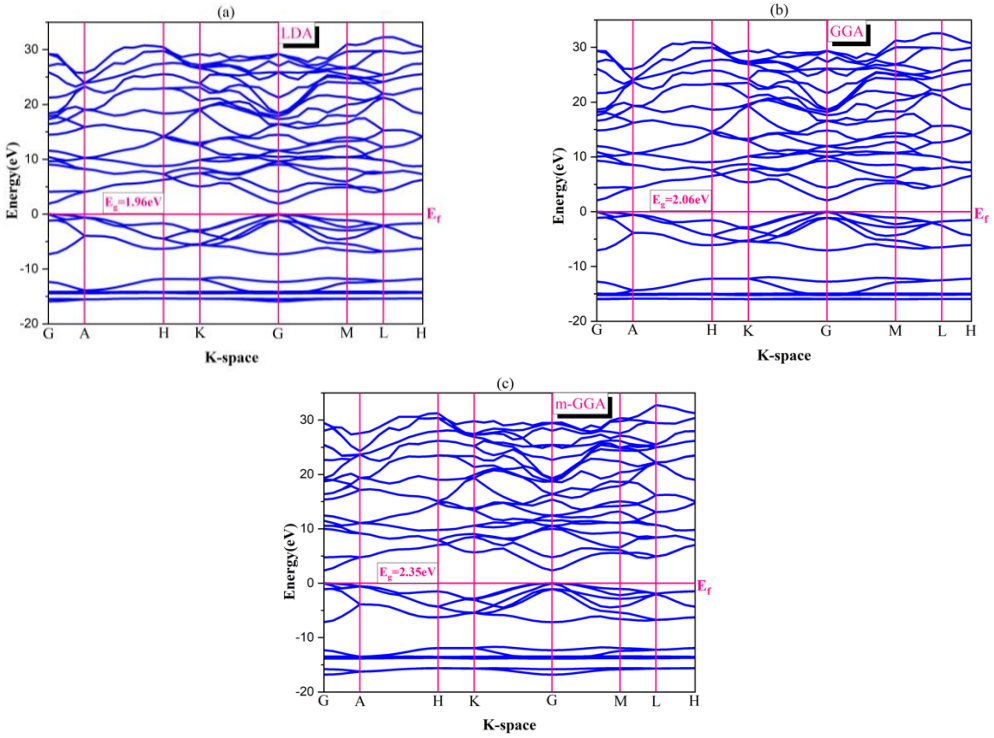


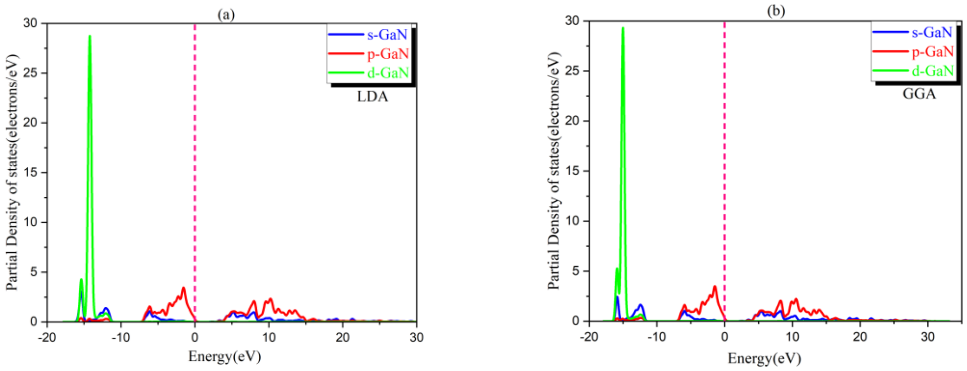

**Figure 2.** Band structure of GaN in the wurtzite phase within (a) LDA, (b) GGA and (c) m-GGA method

**Table 2.** The wurtzite phase energy band gap (Eg) of GaN has been measured by many techniques, including m-GGA, GGA and LDA

| Phase | Approach | $E_g$ (eV) | Reference |
|---|---|---|---|
| **α-GaN** | LDA | 1.962 | Present work |
| | GGA | 2.069 | |
| | m-GGA | 2.354 | |
| | LDA | 2.04 | Qin et al. (2017) |
| | GGA | 1.83 | Magnuson et al. (2010) |
| | Experiment | 3.5 | Yoshikawa et al. (2004) |

### *3.3. Density of State*

The density of states (DOS) refers to the distribution of available energy states in a system, while the partial density of states (PDOS) focuses on the distribution of states within a specific energy range or orbital. In other words, the PDOS provides a more detailed analysis of the DOS by breaking it down into specific energy contributions from different atomic orbitals or molecular orbitals. Figures 3 and 4 show PDOS, TDOS and the Fermi level as a dashed line separating the valence and conduction bands. In Figure 3, the PDOS graph shows the density of states for each energy level within the valence and conduction bands, while the TDOS graph in Figure 4 represents the overall density of states across all energy levels. The Fermi level, indicated by the dashed line, serves as a reference point to distinguish between occupied and unoccupied states. In the energy range from -20 eV to 35 eV, states are plotted. Figure 4(a, b, c) shows typical results for the total DOS of GaN in the wurtzite phase using LDA, GGA and m-GGA, α-GaN has some important properties. LDA or Local Density Approximation, is a simple and computationally efficient method that assumes a uniform electron density throughout the system. GGA or Generalized Gradient Approximation, takes into account the gradient of the electron density, resulting in improved accuracy for some properties. m-GGA or meta-generalized Gradient Approximation, goes a step further by considering not only the electron density and its gradient but also the Laplacian of the density, leading to even more accurate predictions. These different approximations allow for a more comprehensive understanding of the electronic structure of GaN in the wurtzite phase, revealing its unique and significant properties in the P63mc -GaN structure. In Figure 3(b) Ga atom's *p* and *s* electrons are responsible for the majority of its energy levels (ranging from 2.5 to 12.5 electron volts). The smallest contribution comes from the *s* orbital of the N atom; (ii) Among the states from 7.5 eV to Fermi energy, most originate from p electrons of N atoms and small contributions from s electrons; (iii) During the lower energy part of the DOS (in the range of 17.5 to 10 eV), a substantial contribution is generated by the electron s of N and a relatively small contribution comes from the electron p of N. In m-GGA calculation, the intensity is increased and better treatments of the band structure are achieved than in LDA calculation and GGA calculation. The band gap obtained from the DOS plot is consistent with the values determined using GGA and LDA methods, as demonstrated in references (Khan *et al*., 2020; Fan *et al*., 2016).



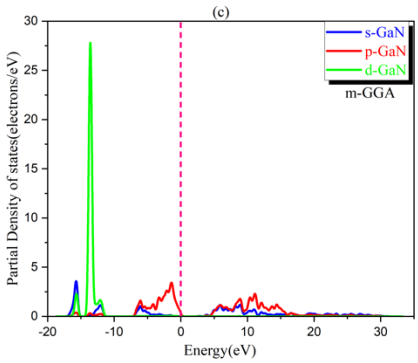



**Figure 3.** The PDOS of the α-GaN, using functional (a) LDA, (b) GGA and (c) m-GGA

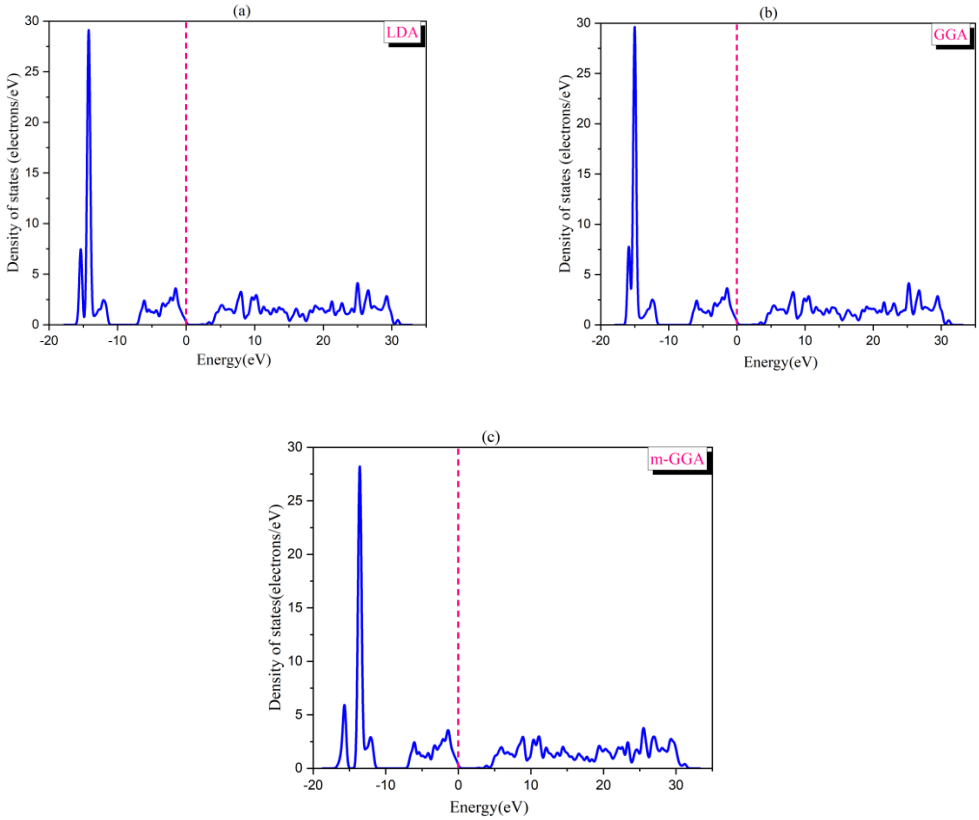



**Figure 4.** The total DOS of α-GaN, using functional (a) LDA, (b) GGA and (c) m-GGA

### *3.4. Optical Properties*

The response of a material to light is heavily influenced by its optical properties, making it necessary to study these properties for optoelectronic purposes. When a photon hits a substance, electrons move from the valence band to the conduction band. The optical response varies between materials due to changes in valence and conductivity bands caused by impurities and defects. The relationship between energy and absorption coefficient can be mathematically described by the absorption spectrum of the material. The absorption spectrum shows how much energy is absorbed by the material at different wavelengths or frequencies. At certain energy levels, called absorption peaks, the absorption coefficient is maximum, indicating that the material absorbs light most

efficiently at those energies (Zaman *et al*., 2022). The graph in Figure 5 shows the absorption spectrum α(ω) of wurtzite-type GaN with LDA, GGA and m-GGA exchange-correlation potentials. By examining absorption coefficients at different energy levels, scientists can learn about the properties and actions of materials in different applications. Absorption in pure GaN starts at 3.5 eV (optical band gap), which is smaller than the electronic band gap. Below the band gap, absorption is close to zero and increases as photon energy increases, reaching about 12.95 eV in the UV region.

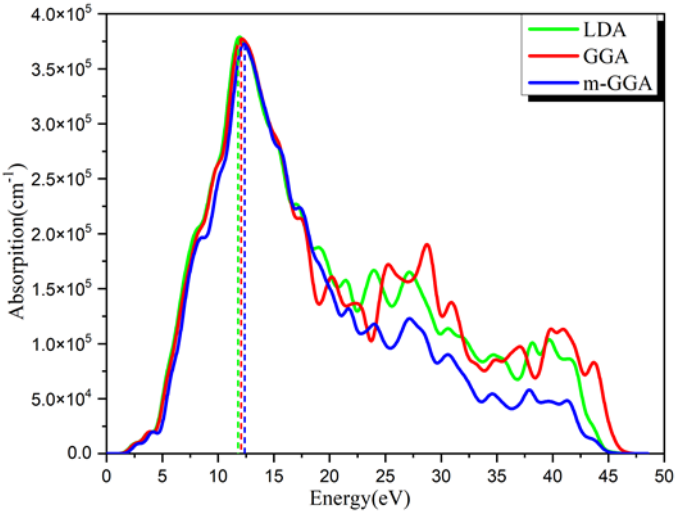



**Figure 5.** Absorption coefficients α(ω) of (green) LDA, (red) GGA and (blue) m-GGA as a function of photon energy. Absorption spectra are plotted versus photon energy

### *3.5. Thermodynamic properties*

Various thermodynamic properties, including Debye temperature, enthalpy, free energy, entropy and heat capacity, were analyzed to explore alterations in thermal characteristics at zero pressure. The Debye temperature (Zhang & Zhang, 2014) signifies the peak mode of vibration of the crystal during phonon vibrations. At zero pressure using the calculated phonon density of states emplying quasi-harmonic approximation. The following equations have been used to calculate the phonon contribution to the Helmholtz free energy F, the entropy E, enthalpy S and the constant-volume specific heat Cv (Tuncel *et al*., 2009):

$$\mathrm{F} = 3nNK_BT \int_0^{\omega_{max}} ln\left\{2sinh\frac{\hbar\omega}{2K_BT}\right\} g(\omega)d\omega \tag{1}$$

$$\mathrm{E} = 3nN\frac{\hbar}{2} \int_0^{\omega_{max}} \omega coth\left(\frac{\hbar\omega}{2K_BT}\right) g(\omega)d\omega, \tag{2}$$

$$\mathrm{S} = 3nNK_B\left[\int_0^{\omega_{max}} \frac{\hbar\omega}{2K_BT}\,\omega coth\left(\frac{\hbar\omega}{2K_BT}\right) - ln\left\{2sinh\frac{\hbar\omega}{2K_BT}\right\}\right] g(\omega)d\omega\,, \tag{3}$$

$$\mathrm{C_v} = 3nNK_B \int_0^{\omega_{max}} (\frac{\hbar\omega}{2K_BT})^2\, csch^2\left(\frac{\hbar\omega}{2K_BT}\right) g(\omega)d\omega\,, \tag{4}$$

$$\theta_D = \frac{h}{K_B}\left[\frac{3m}{4\pi}\left(\frac{N_A\rho}{M}\right)\right]^{1/3} v_m \ . \quad (5)$$

The Planck's constant, denoted by h and the Boltzmann constant, denoted by kB, are used in the expression. The volume of the unit cell is represented by V, while n signifies the number of atoms within a unit cell and $v_m$ indicates the average sound velocity. The average sound velocity, $v_m$, can be calculated using the equation provided (Anderson, 1963).

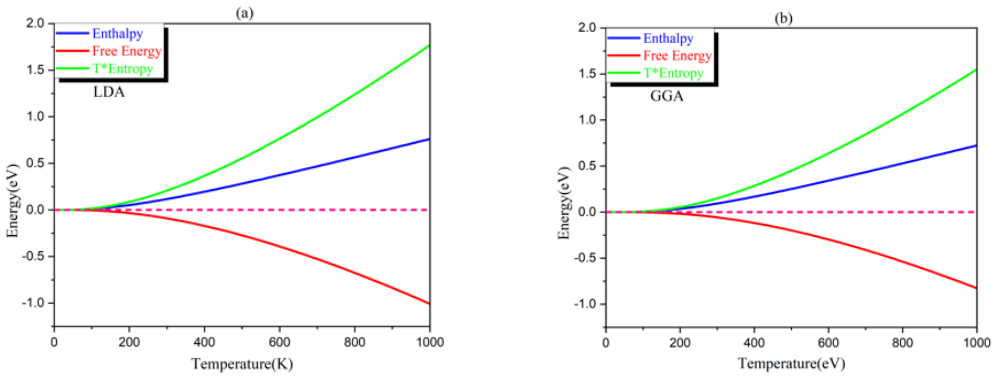
$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\right]^{-\frac{1}{3}} \ . \quad (6)$$

The longitudinal and transverse sound velocities, represented by $v_l$ and $v_t$ respectively, can be estimated by utilizing the values of bulk modulus, B and shear modulus, G. This estimation can be achieved through the application of the following expression (Anderson, 1963).

$$v_l = \left(\frac{B + \frac{3}{4}G}{\rho}\right) \text{ and } v_t = \left[\frac{G}{\rho}\right]^{\frac{1}{3}} \ . \quad (7)$$

Figure 6 illustrates the profiles of the thermodynamic potentials' enthalpy, free energy and the temperature times the entropy term, TS = U − F, with respect to temperature (in K) for α-GaN, utilizing functional LDA, GGA and m-GGA. It can be observed that the enthalpy (solid blue line) shows a nearly linear trend in relation to temperature, while the free energy (solid red line) experiences a slight decrease until 380 K, followed by a linear pattern with increasing temperature. As expected, the term TS (solid green line) demonstrates significant growth as temperature increases.

Thermodynamic potentials, such as enthalpy and free energy, play pivotal roles in understanding the behavior of physical systems. By considering the interplay of these potentials with entropy, scientists can make predictions about the spontaneity and feasibility of processes. As we continue to explore the intricacies of thermodynamics, these concepts will remain fundamental in our quest for a deeper understanding of nature's laws.



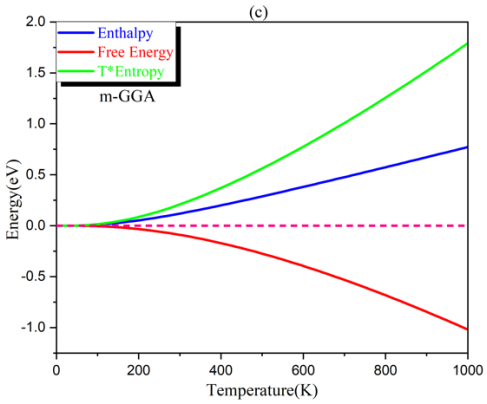



**Figure 6.** Shows the enthalpy, free energy and entropy of the GaN wurtzite phase with using (a) LDA, (b) GGA and (c) m-GGA, respectively all calculations in the range 0–1000K

The heat capacity obtained through the LDA, GGA and m-GGA techniques is illustrated in Figure 7. A clear power-law temperature correlation is observable for the heat capacity at lower temperatures. The power-law exponent calculated for the two GaN crystals is around 3, consistent with the Debye heat capacity theory. Apart from this, the heat capacities of LDA at 300 K were calculated to be 22.5 J $mole^{-1}K^{-1}$, GGA gave 23.6 J $mole^{-1}K^{-1}$ and m-GGA obtained a value of 24.3 J $mole^{-1}K^{-1}$. The experimental heat capacity of wurtzite GaN being 23 J $mole^{-1}K^{-1}$ at 300 K, the values of the fitted parameters are close to those of the 300 K range (Danilchenko *et al*., 2007). This means that the GaN crystal has an effective heat capacity of 23.6 J $mole^{-1}K^{-1}$, known as the Dulong–Petit limit. This value is characteristic of materials at elevated temperatures. It obviously comes to our view that the thermal capacity, the heat capacities of GaN crystals do not show any variation from 0 to 1000 K, signifying that the structure of crystal in GaN does not influence it. The heat capacity of wurtzite GaN is affected by several parameters not the least of which are those due to lattice vibrations, crystal distortion and the existence of impurities and defects. In addition to that phonon mean free path that gives the ability of lattice vibrations to travel an expected distance before the occurrence of scattering also influences the heat capacity of wurtzite GaN.

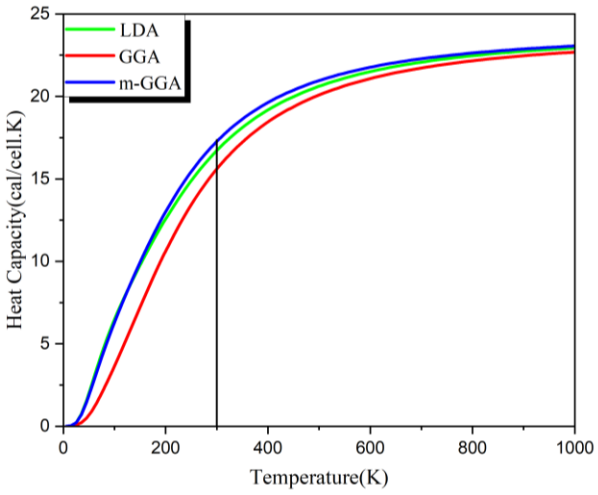



**Figure 7.** Depicts the heat capacity determined using the LDA, GGA and m-GGA methods

The relationship between the Debye temperature and temperature is illustrated in Figure 8. The Debye temperature serves as an indicator of the bonding strength among atoms and consequently correlates with the material's hardness. Typically, a greater Debye temperature signifies a higher level of hardness (Ravindran *et al*., 1998). When examining the dependence of the Debye temperature on temperature under zero pressure conditions, it becomes evident that the GaN crystal undergoes softening. However, the application of pressure can counteract this softening effect. The Debye temperature ΘD at room temperature is determined to be 395 K. It is observed in Figure 8 that pressure has a more pronounced impact on ΘD compared to temperature. Additionally, the Debye temperatures of GaN exhibit variability, with previous research indicating values ranging from 586 K to 898 K for wurtzite GaN (Roder *et al*., 2005). In the current investigation, the calculated Debye temperatures for wurtzite GaN are 845 K, 916 K and 788 K for LDA, GGA and m-GGA, respectively, at 300 K.

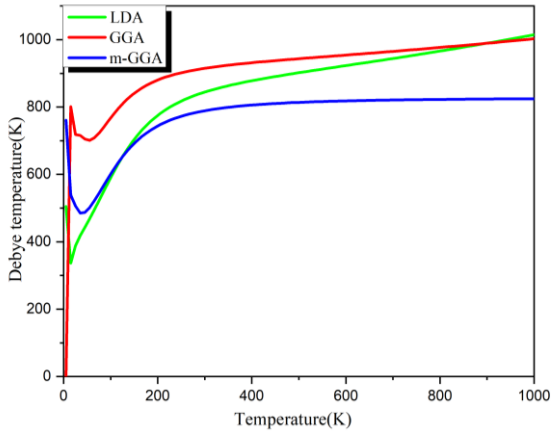



**Figure 8.** The value of Debye temperature using LDA, GGA and m-GGA

## 4. Conclusions

We present a detailed investigation of the wurtzite GaN's structural, electronic, optical and thermodynamic properties in this work the LDA, GGA and m-GGA approximations were used in the computation of the pseudo-potential plane waves (PP-PW), which is a method based on the theory of the density functional (DFT) and implemented in the CASTEP code. The calculation of the electronic band of this compound reveals a direct band gap. In contrast, the density of total and partial states (DOS and PDOS) as well the optical constants, α(ω) have also been computed. The quasi-harmonic approximation was utilized to compute the temperature dependence of a few parameters including: Debye temperature, enthalpy, free energy, entropy and heat capacity for wurtzite GaN. Two different methods, such as LDA and GGA approaches were used in this research in order to obtain the energy band gap in which the electronic band gap and the gap between the valence band and the conduction band were 1.962eV and 2.069eV respectively. Also, the result of the m-GGA showed a band gap of 2.354 eV. Both the LDA and GGA methods have underestimated energy band gap, however, the m-GGA method has resolved this conflict and provides results that are in close agreement with the experimental studies. In addition, m-GGA method has been demonstrated to be efficient because of its capability to accurately describe the electronic states. In the last, the conclusion is made that the m-GGA is an exceptional tool for computing the essential electronic structure of wurtzite GaN which means that the material is appropriate for

optoelectronic applications. Not only the simulation is acknowledged to have close relationship to the experimental and theoretical results, but it is also considered to be a very good prediction for the investigation that may be conducted in the immediate future.

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