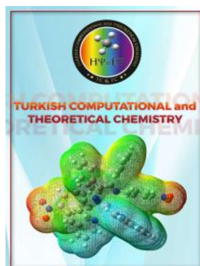

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Structural and electronic properties of GaN: Ab initio study within LDA and LDA+U methods

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Abstract: *Structural and electronic properties of the GaN were simulated based on Density Functional Theory implementing Local Density Approximation methods. Hubbard U correction gives us an opportunity to find the correct energy gap for GaN in agreement with known experimental results. Choosing more accurate investigation methods leads to calculating accurate electronic band structure and in the future predicting some physical properties of related material. The bottom of the conduction band and the top of the valence band are formed mainly by p-orbitals of host Ga and N atoms. The present study shows the direct band gap character of GaN with a wurtzite structure.*

Keywords: Gallium Nitride, LDA, LDA+U, electronic structure, density of states

1. Introduction

Nowadays, III-nitrides such as Gallium Nitride (GaN) especially, are interesting for basic scientific research and possible technical applications. This compound is a wide band gap material and can be synthesized using molecular beam epitaxy, metalorganic chemical vapor deposition, and hydride vapor-phase epitaxy (HVPE) methods [1]. Due to its unique physical properties, GaN has attracted the attention of researchers according to its technical employments, such as quantum-point lasers, transistors, lasers that range from red to ultraviolet (UV), etc. [2-5]. Wurtzite-type configuration is the thermodynamically stable phase with an energy gap close to 3.4 eV [6-8].

The analysis of literature on electronic structure of GaN shows that the theoretically computed band gaps [8-11] were underestimated with experimental results [6-8]. These studies reported results based on the DFT (Density Functional Theory) [12] employing LDA (Local Density) [13] or GGA (Generalized Gradient Approximations) [14] method. It is known that ab initio methods are infamous for simulating too narrow energy gaps for semiconductors when computed from the Kohn-Sham energy eigenvalues. The Hubbard U energy [15] will then suggest a simple investigation method to correctly obtain the behavior of highly correlated compounds. Using the Hubbard U approach and implementing LDA (or GGA) methods, a DFT-LDA(GGA)+U scheme is built, which is computationally advantageous for correct simulations of electronic properties. By successfully calculating the accurate band structure of the studied compound, can extend the study of electronic and magnetic properties of GaN. The problem for GaN is that the LDA predicts that the gallium 3d-orbitals overlap with the nitrogen 2s-states forming two sets of bands. Recently, the experimental results have shown that the 3d-states of the Ga lay several eV below the 2s-states of N [16-20].

2. Computational Method

DFT is a successful theory to calculate the electronic structure of atoms, molecules, and solids. Its goal is the quantitative understanding of material properties from the fundamental laws of quantum mechanics. Traditional electronic structure methods attempt to find approximate solutions to

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the Schrödinger equation of N interacting electrons moving in an external, electrostatic potential (typically the Coulomb potential generated by the atomic nuclei). However, there are serious limitations of this approach: (i) the problem is highly nontrivial, even for very small numbers N and the resulting wave-functions are complicated objects, (ii) the computational effort grows very rapidly with increasing N, so the description of larger systems becomes prohibitive [12].

The foundation of DFT is the Kohn-Sham theorem. The Kohn-Sham equations are at the heart of modern DFT. They have the form of the single-particle Schrödinger equation

$$\left[-\frac{\nabla^2}{2}+\upsilon_s(r)\right]\varphi_i(r)=\varepsilon_i\varphi_i(r) \quad (1)$$

where $\upsilon_s(r)$ is the single-particle potential. The density can then be computed from the N single-particle orbitals occupied in the ground state Slater determinant

$$n(r)=\sum_i^{occ}\left|\varphi_i(r)\right|^2 . \quad (2)$$

The central idea of the Kohn-Sham scheme is to construct the single-particle potential $\upsilon_s(r)$ in such a way that the density of the auxiliary non-interacting system equals the density of the interacting system of interest. To this end one partitions the Hohenberg-Kohn functional in the following way

$$F[n]=T_s[n]+U[n]+E_{xc}[n], \quad (3)$$

$$U[n]=\frac{1}{2}\int d^3r\int d^3r'\frac{n(r)n(r')}{|r-r'|}$$

(4)

where is the classical electrostatic energy of the charge distribution n(r), and $E_{xc}[n]$ is the so-called exchange-correlation energy which is formally defined by

$$E_{xc}[n]=T[n]+V_{ee}[n]-U[n]-T_s[n] . \quad (5)$$

$E_{xc}[n]$ is a universal functional of the density, i.e., it has the same functional form for all systems. On one hand this is a promise because an approximate functional, once constructed, may be applied to any system of interest. On the other hand this is a challenge because a good approximation should perform equally well for very different physical situations. Both the promise and the challenge are reflected by the fact that the simplest of all functionals, the so-called LDA [13] has remained the approximation of choice for quite many years after the formulation of the Kohn-Sham theorem. In LDA [13], the exchange-correlation energy is given by

$$E_{xc}^{LDA}[n]=\int d^3r \quad n(r)e_{xc}^{unif}(n(r)) \quad (6)$$

where $e_{xc}^{unif}(n)$ is the exchange-correlation energy per particle of an electron gas with spatially uniform density *n*. The LDA is expected to be a good approximation for spatially slowly varying densities. Although this condition is hardly ever met for real electronic systems, LDA has proved to be remarkably accurate for a wide variety of systems.

One of the standard uses of DFT [12] in solid state physics is the calculation of band structures. Usually one interprets and compares the Kohn-Sham band structure directly with experimental energy bands. Strictly speaking this interpretation has no sound theoretical justification since the Kohn-Sham eigenvalues are only auxiliary quantities. Experience has shown, however, that LDA band structures are often rather close to experimental ones, especially for simple metals. On the other hand, a well-known problem in semiconductors and insulators is that LDA [13] seriously underestimate the band gap. Nevertheless, the last progress of LDA functional and using Hubbard U semiempirical corrections have given us an opportunity to determine correct band gaps of materials.

In this study, first-principles simulations were carried out implementing the Atomistic ToolKIt (ATK) code (http://quantumwise.com/) and this is a software for atomic-scale modeling and simulation of nanosystems. ATK combines density functional theory (DFT) with non-equilibrium Green's functions for first-principles electronic structure and transport calculations of molecules, periodic systems etc. Based on the DFT and LDA methods, we simulated the structural and electronic properties of the GaN. The Monkhorst-Pack scheme [21] was set to a 7×7×7 grid and 172

symmetry-reduced *k*-points sampling in the irreducible part of the Brillouin zone integration.

Electron-ion interactions are accounted for by norm-conserving Frits-Hubbard-Institute (FHI) [22] pseudopotentials and Double Zeta Polarized (DZP) basis set. The electron kinetic cutoff energy was taken equal to 75 Ha (i.e. 150 Ry) was employed throughout the calculations which were tested to be fully converged with for total energy.The three electrons for Gallium [Ar] $+4s^2$ $4p^1$ and five electrons for Nitrogen [He] $+2s^2$ $2p^3$ were treated as valence electrons in recent calculations. At the initial step, the equilibrium configuration of GaN was found, and the total energies of structures were geometrically optimized with respect to the structure parameters. The initial structural parameters for GaN were set based on experimental dates from reference [23]. For the build structure of GaN, the initial structure parameters were used taken from Ref. [23]. The calculation convergence criterion in the case of the optimization of GaN was relaxed and geometrical optimized due to no higher than 0.001 eV/Å force and 0.001 eV/Å^3 stress tolerances.

To calculate an accurate band gap for GaN, we implemented the Hubbard U semiempirical corrections for Ga 5*d*- (5 eV) and N 4*p*-orbitals (4.8 eV). The Hubbard U correction is applied using the simplified approach according to Dudarev et al. [24], which corresponds to the case J=0 in the more elaborate expression by Lichtenstein et al. [25].

Note that, for all calculations, the convergence of the plane-wave basis set cutoff energy and Brillouin zone integration *k*-point sampling of GaN were tested.

3. Results and discussion

3.1. Structural properties of GaN

The investigated semiconductor compound GaN has a hexagonal structure with space group $P6_3mc$ (No.186) and with four atoms per primitive unit cell. In this compound, Ga and N atoms occupy Wyckoff positions 2b with fractional coordinates [26]. The two gallium atoms occupy positions (1/3, 2/3, 0) and (2/3, 1/3, 1/2), and two nitrogen atoms occupy positions (1/3, 2/3, u) and (2/3, 1/3, u+1/2). This compound can be depicted as alternating planes of tetrahedral coordinated with N^{3-} ions surrounded by Ga^{3+}, generating [GaN_4] clusters and stacked alternately along the *c*-axes [27]. GaN has two external lattice parameters and one internal coordinate corresponds to the Nitrogen position with consideration to Ga. For all calculations were carried out, the geometry optimization process of compounds. The fractional atomic coordinates [23] used for present calculations and obtained distances between host atoms were given in Tables 1 and 2.

In Table 2, for comparison, we included the previously experimentally [23, 28] and theoretically [10, 29] reported values for distances Ga-N and Ga-Ga. The optimized values of bond lengths are closer to theoretical and experimental dates.

For the current first-principle calculations we have relaxed all GaN wurtzite structures as shown in Fig. 1.

The first-principles obtained structure parameters using LDA and LDA+U approximations, comparing with other known theoretical [8-11, 27, 29-32] and experimental [6-8, 23, 26, 28] dates, are listed in Table 3. The optimized values of structure parameters exhibit good agreement with previously obtained results. Both LDA and LDA+U GaN bulk parameters are in agreement with the experimental dates [6-8, 23, 26, 28]. The DFT-LDA+U obtained lattice parameters (*a* and *c*) are smaller than the experimental results. As seen from the Table 3, the DFT-LDA and LDA+U computed parameters are an estimation of experimental dates [6-8, 23, 26, 28], with 0.1÷0.6 % (for *a*), 0.18÷0.9 % (for *c*) and 0.3÷1.1 % (for *a*), 5.9÷6.6 % (for *c*) difference for lattice parameters of GaN wurtzite, respectively.

Note that, Tables 2 and 3 represent the average bond lengths and lattice constants after the optimization process.

Table 1. Positions (primitive cell) of atoms used for present calculations.

Atoms	Positions		
	X	*y*	*z*
Ga	0.33333	0.66667	0
Ga	0.66667	0.33334	0.5
N	0.33333	0.66667	0.385
N	0.66667	0.33334	0.885

Table 2. The first-principles calculated bond length lists for the GaN compound.

Bond length, Å	DFT-FHI-DZP		Theor.		Exper.	
	LDA	LDA+U	[10]	[29]	[23]	[28]
Ga-N	1.96	1.94	1.9571	1.962	1.99	1.93
Ga-Ga (N-N)	3.20	3.05	-		3.17	-

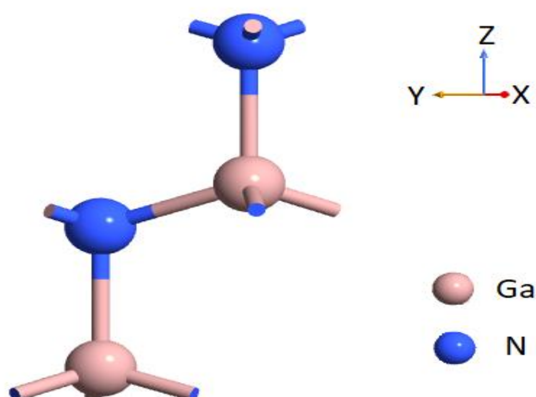


Fig. 1. The structural configuration of GaN wurtzite.

Table 3. First-principles optimized bulk parameters for GaN wurtzite structure. A comparison between the present lattice constants and other known results.

Comp. Code	*a,*	*c*	*c/a*	*u*	Refs.
ATK, LDA	3.200	5.214	1.629	0.380	This work
ATK, LDA+U	3.169	4.878	1.539	0.391	This work
CRYSTAL17, B3LYP	3.212	5.204	1.620	0.377	Theor.[27]
CRYSTAL03, B3LYP	3.193	5.174	1.620	0.379	Theor.[29]
PPPW, LDA	3.18	5.183	1.63	0.3765	Theor.[30]
PPPW, GGA	3.25	5.298	1.63	0.3765	Theor.[30]
PPPW, LDA	3.193	5.218	1.634	0.376	Theor.[11]
FP-LAPW, GGA	3.18	5.166	1.625	0.376	Theor.[9]
VASP-PAW, GGA	3.1999	5.2186	1.630	-	Theor.[10]
PPPW, LDA	3.193	5.218	1.634	0.376	Theor.[11]
PPPW, GGA	3.245	5.296	1.632	0.3762	Theor.[11]
HF, LDA	3.199	5.176	1.618	0.380	Theor.[31]
CRYSTAL92,HF	3.2011	5.1970	1.6235	0.3775	Theor.[32]
WC-GGA	3.1904	5.1907	1.6270	-	Theor. [8]
WC-GGA+U (U_d(Ga)=10 eV)	3.1565	5.1324	1.626	-	Theor. [8]
X-ray spectroscopy	3.1921	5.1842	1.6241		Exper.[8]
Optical-absorption measurements	3.185	5.189	1.629	-	Exper.[7]
XRD data	3.18	5.166	1.624	0.385	Exper.[23]
XRD data	3.181(3)	5.184(4)	1.629	0.337(2)	Exper.[26]
X-ray analysis	3.189	5.185	1.625	-	Exper.[6]
Reactive Magnetron Sputtering	3.2039	5.2041	1.624	0.398	Exper.[28]

Table 4. The DFT-LDA result of the band gap for GaN bulk structure

Comp. Code	Band gap, eV	Refs.
ATK, LDA	2.0	This work
CRYSTAL03, B3LYP	3.87	Theor.[29]

PPPW, GGA	1.45	Theor. [11]
PPPW, LDA	1.76	Theor.[11]
FP-LAPW, GGA	1.992	Theor.[9]
VASP-PAW, GGA	1.818	Theor.[10]
WC-GGA	1.83	Theor.[8]
Reactive Magnetron Sputtering	3.2	Exper.[28]
Optical-absorption measurements	3.39	Exper.[6]
	3.41	Exper.[7]
SXE-SXA spectra	3.4	Exper.[8]

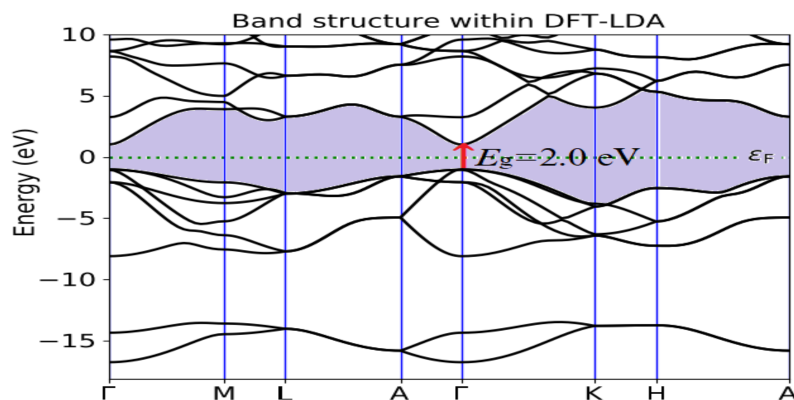


Fig. 2. First-principles calculated band structures of GaN within the LDA (E_g=2.0 eV) method. Fermi energy is set to 0 eV and shown with a dotted line.

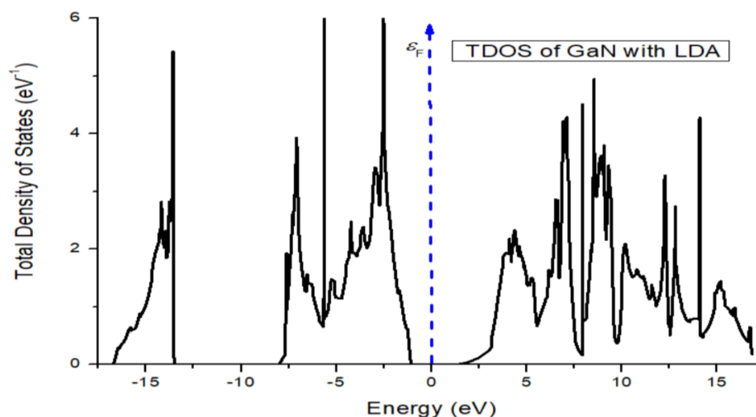
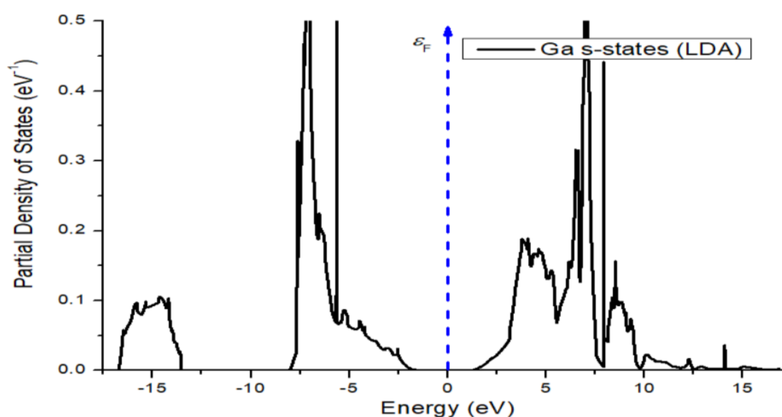
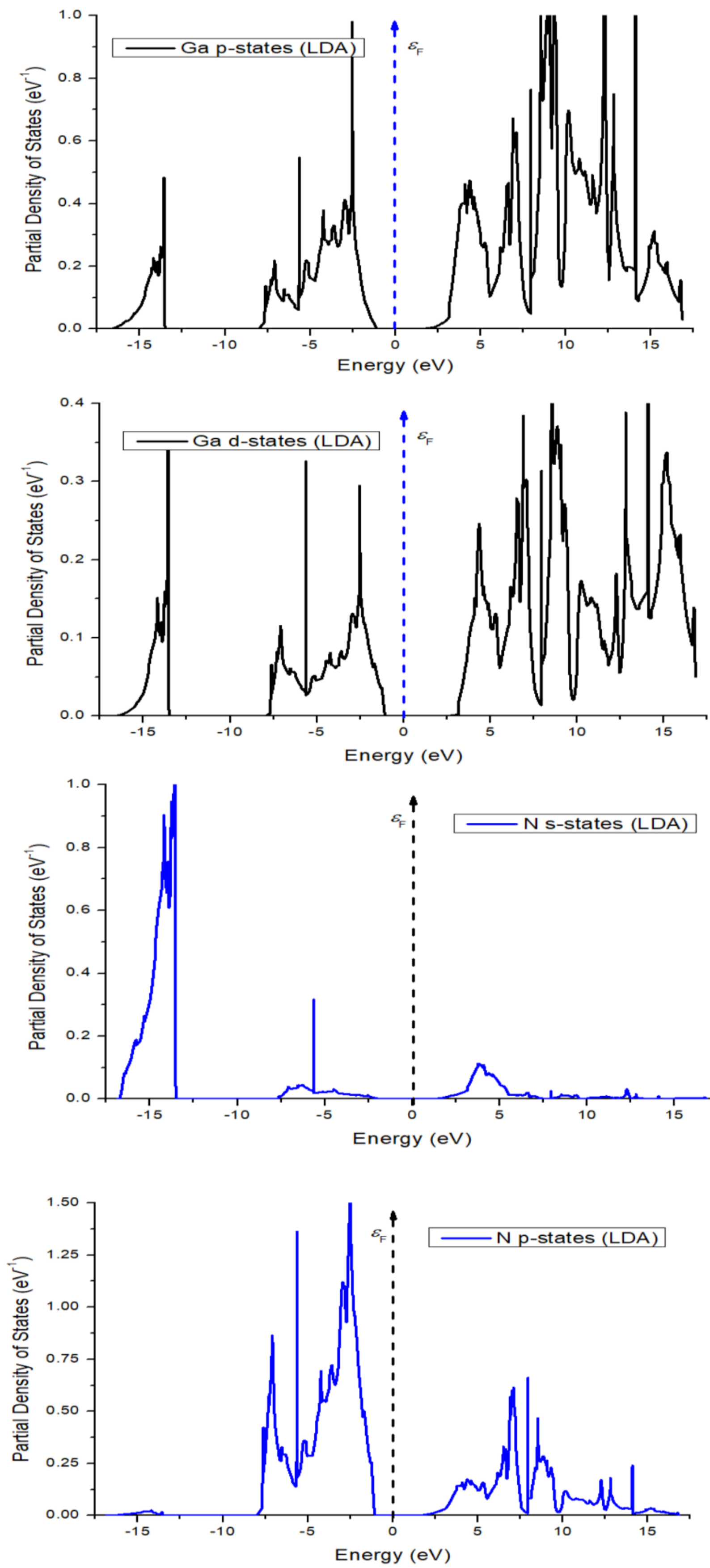


Fig. 3. First-principles calculated TDOS diagram of GaN within LDA. Fermi energy is set to 0 eV and shown with a dotted line.




Ga p-states (LDA)
ε_F
Partial Density of States (eV^{-1})
Energy (eV)
Ga d-states (LDA)
ε_F
Partial Density of States (eV^{-1})
Energy (eV)
N s-states (LDA)
ε_F
Partial Density of States (eV^{-1})
Energy (eV)
N p-states (LDA)
ε_F
Partial Density of States (eV^{-1})
Energy (eV)

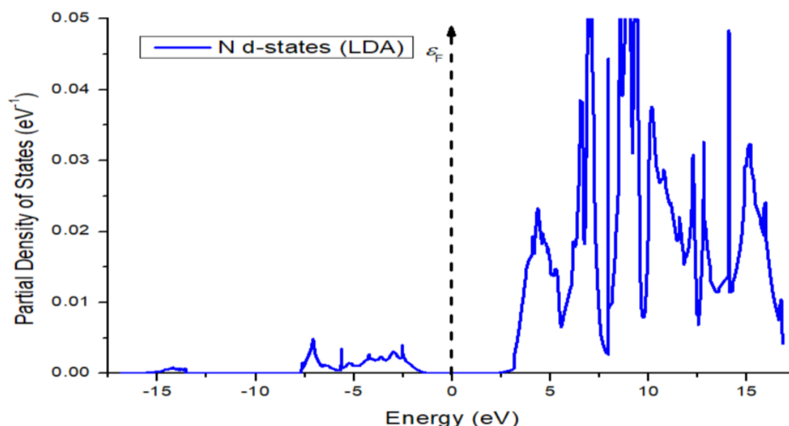


Fig. 4. First-principles calculated PDOS diagrams of GaN within the LDA method. Fermi energy is set to 0 eV and shown with a dotted line.

Table 5. The result of the band gap for the GaN with LDA+U.

Comp. Code	Band gap, eV	Refs.
ATK, LDA+U (U_d(Ga)=5 eV; U_p(N)=4.8 eV)	3.36	This work
WC-GGA+U (U_d(Ga)=10 eV)	2.4	Theor.[8]
SXE-SXA spectra	3.4	Exper.[8]
Optical-absorption measurements	3.39	Exper.[6]
	3.41	Exper.[7]

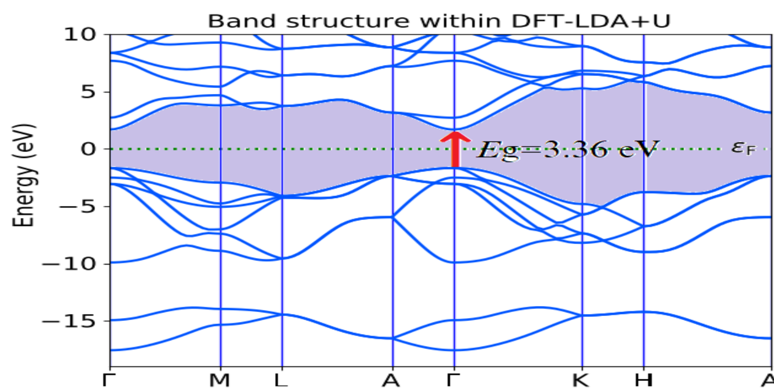


Fig. 5. Calculated band structure of the GaN within the LDA+U method (E_g=3.36 eV). Fermi energy is set to 0 eV and shown with a dotted line.

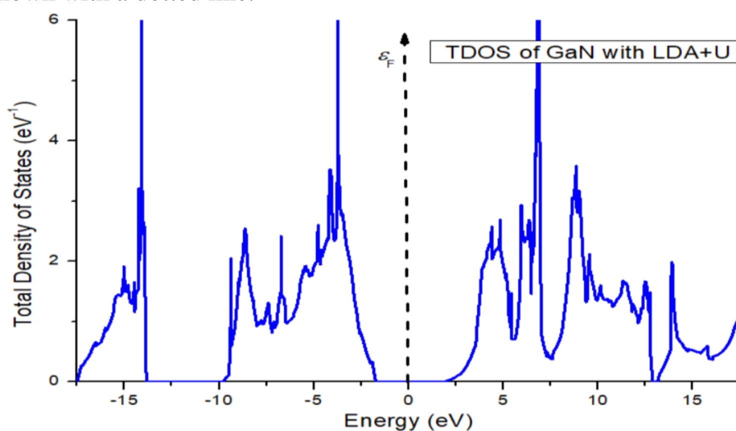
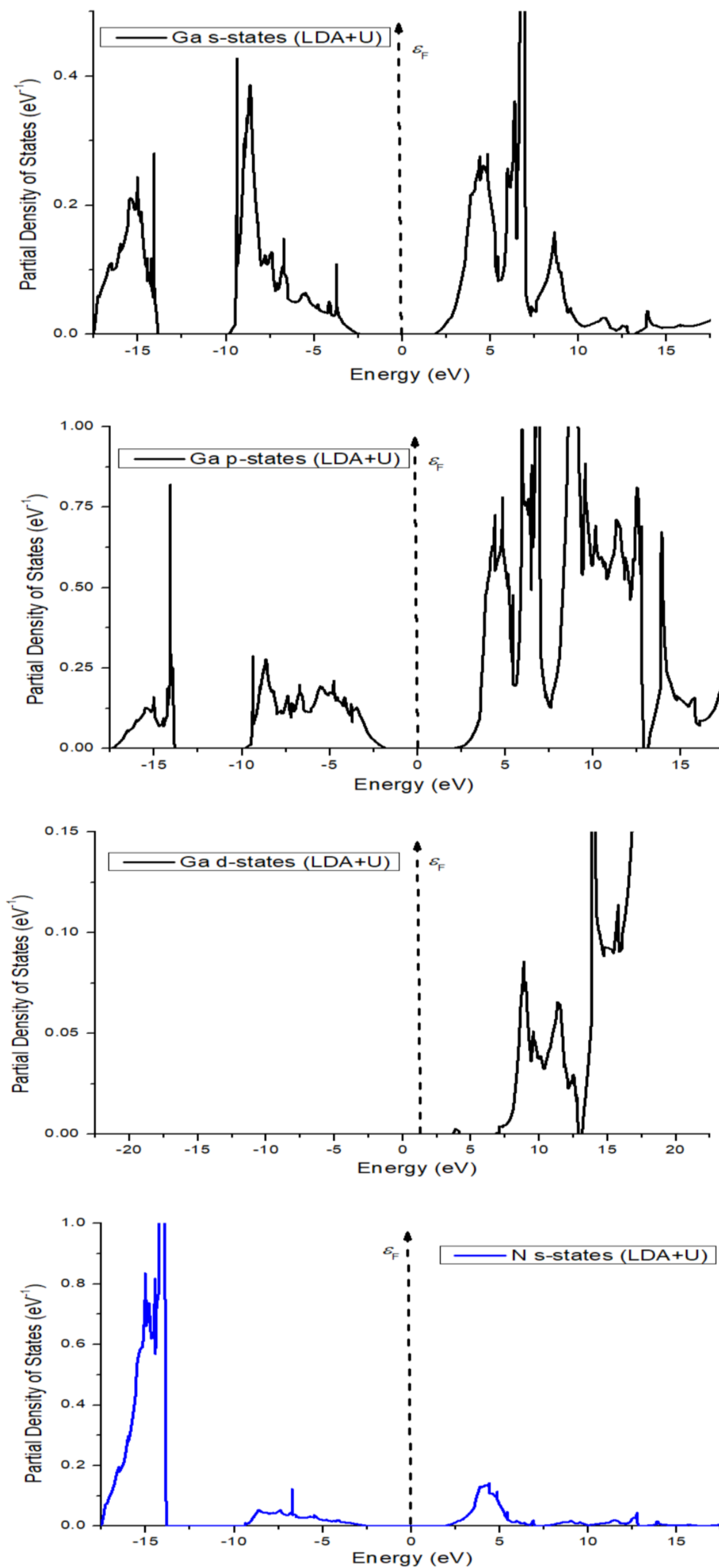


Fig. 6. Calculated TDOS diagram for the GaN within the LDA+U. Fermi energy is set to 0 eV and shown with a dotted line.



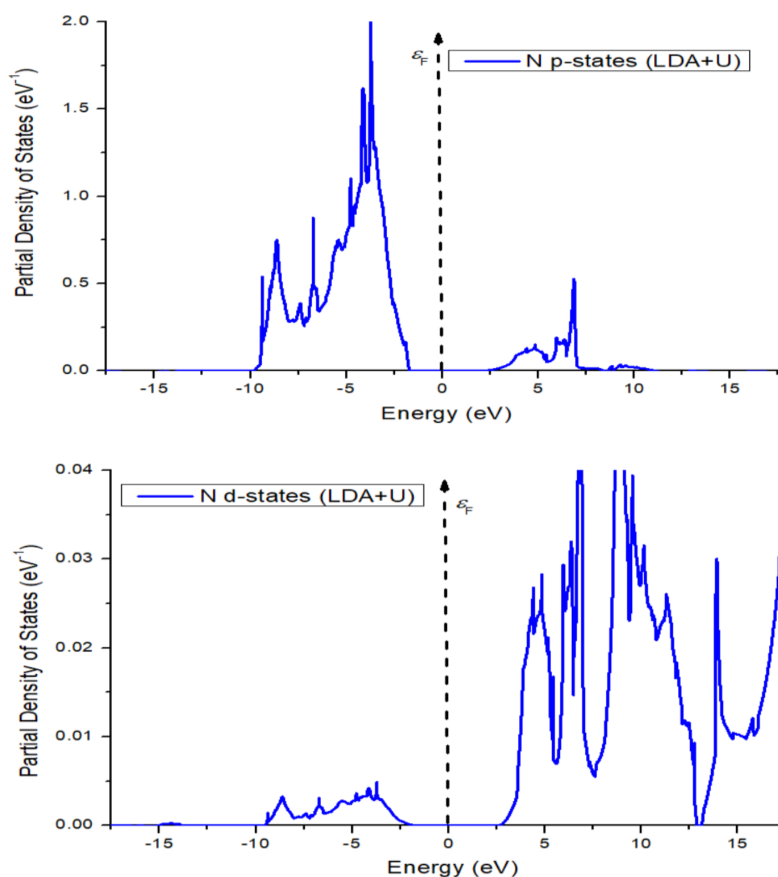


Fig. 7. Calculated PDOS of the GaN within the LDA+U. Fermi energy is set to 0 eV and shown with a dotted line.

3.2. Electronic properties of GaN within the DFT-LDA method

In this section, we have simulated the electronic structure within LDA and we obtain a smaller gap than experimental results [6-8, 28]. In Refs. [6, 7] from optical-absorption measurements experimentally obtained band gaps of GaN are 3.39 and 3.41 eV, respectively. From Soft X-ray absorption (SXA) and emission (SXE) spectroscopy measurements found the value of the energy gap is 3.4 eV. Mazini et al. [29] computed the electronic structure of GaN using CRYSTAL03 program package and implementing B3LYP functional and obtained a larger band gap value (3.87 eV) compared to known experimental results [6-8, 28]. Other works [8-11, 29] devoted to electronic structure of GaN reported results of gaps (from 1.7 to 2.4 eV) are underestimated than experimental. In Table 4, we listed our DFT-LDA result for the band gap of GaN wurtzite, for comparison including other results.

From Table 4, the values of band gaps of all DFT calculations (apart from Ref.[29]) are smaller than experimental results, when non-implementing Hubbard U. The obtained results for the GaN compound are represented in Fig. 2. Fermi energy (ε_F) is set to zero and shown with a horizontal dotted line. The LDA computed electronic structures of GaN we obtained that the energy gap is 2.0 eV, which is ~1.4 eV underestimated known experimental results (3.4 eV) [6-8].

Figs. 3 and 4, show the results of total and partial DOS diagrams of GaN with LDA. Due to the DOS calculations, we can divide the valence band (lower and upper) into two parts. DFT-LDA simulations show that the lowest valence bands are located in the energy range from -16.7 to -14.4 eV and are formed with nitrogen 2*s* orbitals. The upper valence bands are separated from lower bands from -8.1 to -1.0 eV, which is mainly formed by nitrogen 2*p*-orbitals. The minimum of the conduction band is mainly formed by gallium 4*p* in character.

3.3. Electronic properties of GaN with LDA+U

Electronic properties of materials are a powerful tool for understanding semiconductor devices

because they provide qualitative solutions to the semiconductor equations. However, the band structure is responsible for the explanation of the electrical properties of a material.

In section 3.3, we gave the results of simulations using the LDA, and we obtained a smaller band gap with comparison experimental dates. We found only one research work [8] devoted to study of the electronic structure of GaN implementing Hubbard U energy (U_d(Ga)=10 eV) for Ga 3*d* states. The authors [8] showed that an energy gap opened at the point by 0.57 eV, and became 2.4 eV, which is ~1 eV smaller than known experiment. It is known that the DFT+U calculations required a value for U correction in the range from 3 to 6 eV [33] to reproduce the experimental dates. However, implementing large values for U corrections leads to significant change, i.e. the parameters of the unit cell are increasing with increasing the U, due to the Coulomb repulsion increase [34].

In this section, we have simulated the band structure using LDA and implementing semiempirical corrections (LDA+Hubbard U) [33]. However, recent advances in Hubbard U corrections for the *d*-states of Gallium (5.8 eV) and *p* orbitals for Nitrogen (4.8 eV) have enabled us to compute an accurate gap corresponding to experimental dates of GaN semiconductor compound. The computed band gap for GaN is shown in Table 5 and for comparison including other DFT results taken from Ref. [8] and experimental dates.

Fig. 7, represents the PDOS of s, p, and d-states of host atoms. The results of simulations plotted in Figs. 5 and 6, we observe two parts in the valence band on the band structure and TDOS diagrams of the GaN compound. The bands from -17.6 to -14.9 eV are formed from the nitrogen 2s levels and separated from valence bands from -9.9 to -1.7 eV, which are mainly formed by nitrogen 2p states. The lower conduction bands are treated mainly by gallium 4p states. The top of the valence band and the bottom of the conduction band consist of p-orbitals of host atoms.

4. Conclusions

Choosing an accurate investigation method we have studied the structural and electronic properties of GaN. We are shown that using the LDA gives a small gap, which is ~1.4 eV underestimated LDA+U, and known experimental results. However, implementing Hubbard U semiempirical energy corrections enables us to find the correct band gap for GaN with large energy gaps. The results of simulations show that the lowest and upper valence bands are derived from the nitrogen s- and p-states. The bottom of the conduction band is treated mainly by gallium p orbitals.

The results of this paper may be valuable for alloyed and doped Ga-based applications in electronic, optoelectronic, nanoelectronic, and spintronic devices in the future.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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