PHYSICS AND CHEMISTRY OF SOLID STATE
V. 24, No. 4 (2023) pp. 714-721
Section: Physics

DOI: 10.15330/pcss.24.4.714-721

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ФІЗИКА І ХІМІЯ ТВЕРДОГО ТІЛА
Т. 24, № 4 (2023) С. 714-721
Фізико-математичні науки

PACS: 71.15.Dx ISSN 1729-4428

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Assessing the Effect of Electronic Pseudopotentials and Relativistic Treatments on the Structural and Electrical Properties of GaN: a DFT Study

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Applying the principle of Density functional theory, we can calculate various parameters like lattice constant, band gap, band plot, dielectric function plot, refractive index plot, conductivity plot, density of state plot, loss function etc. of GaN. In this work, we use different electronic pseudopotentials with different relativistic treatment studied using Local density approximation functional (LDA-CAPZ) within DFT for GaN. We used to calculate the energy values, lattice parameters change after geometry optimisation and plot the band energies. Electronic structure calculations results are compares taking different electronic pseudopotentials of different cut-off energy having different relativistic approaches. The Density of state plot and partial density of states plot help to studied more about the electronic as well as magnetic characteristics of the GaN sample. Here, we also compare the advantages and disadvantages of different pseudopotentials with different relativistic approaches of the sample. Energy level distribution and partial density of states were compared for all the pseudopotentials with different relativistic treatments, providing insight into the orbital contributions of electrons to the density of levels. Our study provides a deeper understanding into the impact of electronic pseudopotentials and relativistic treatments on the electronic and structural properties of GaN.

Keywords: DFT, LDA, Pseudopotentials, Relativistic Treatments

Received 22 August 2023; Accepted 13 December 2023.

Introduction

In the field of semiconductor research, the study of special materials and their electronic properties is very important for technological progress. Gallium nitride (GaN), a semiconductor material widely used in optoelectronics and high-power electronics. Density functional theory is used to understand the electronic and structural properties of bulk and nano GaN [1-2]. Despite the well-established principles governing semiconductors, the nuanced effects of electronic pseudopotentials and relativistic treatments on the structural and electrical properties of GaN remain an area of active investigation. Some semiconductors like ZnS (3.6eV), GaN (3.4eV), ZnO (3.37eV) have more than 3eV band gap known as wide band gap semiconductor [3]. DFT methods use some of the approximation methods like Local density approximation-LDA [4], Generalized Gradient approximation-GGA [5], Predew-Bruke-Ernzerhof -PBE [6], PW91 [7] to studied the structural, magnetic and optical traits of materials.

In this work, the main objective is to find the appropriate electronic pseudopotentials with different relativistic approximation to study the electronic and magnetic properties of GaN. For all the calculations, we use the LDA-CAPZ functional as it gives better results [8]. Band gap calculations with band plot done in this work. Energy density states distribution and partial density of energy states plot draw and compared among pseudopotentials.

I. Computational methods

Most popular and dependable method is density functional theory which is *first principle* approach of

computation. It is used to examine the properties of materials theoretically. In this piece of work, we used first principle total energy code to calculate the electronic structure. We use CASTEP [9] module in Biovia for this calculations. LDA is one local exchange correlation functional exist in CASTEP and three corrected gradient exchange correlational functional GGA in CASTEP. Also a set of self-consisted total energy calculations nonlocal function exist in CASTEP calculations. In LDA, CA-PZ only local function available which based on Ceperley and Alder (1980) [10] data which parameterised by Perdew and Zunger (1981) [11]. Here the calculations for DFT done with LDA CAPZ functional. For calculations, we taken valence electrons of GaN. The interaction with core and valence electrons pick up by different pseudopotentials. Dassault systems BIOVIA material studio [12] is used for modelling and structure calculations to study the properties of materials. It is used in Material science, physics and chemistry for modelling and simulation.

In this work, we used different pseudopotentials with different cut-off energy. OTFG ultrasoft Pseudopotential having Cutoff Energy 517 eV. For OTFG norm conserving Pseudopotential, the Cutoff Energy is 1115.7 eV. Ultrasoft Pseudopotential having Cutoff Energy 295 eV and norm conserving Pseudopotential has Cutoff Energy 800 eV. The K-point grid taken as 5 ×5 ×4 in all calculations. The energy bands and state densities were displayed after the single particle equations developed by Kohn and Sham [13] were solved. Band energies, density of state and band gap calculations done for hexagonal GaN. GaN has wide band gap of 3.4 eV. GaN has tetrahedral coordinate geometry with lattice dimension of a=b=3.216 Å, c=5.240 Å. GaN is wurtzite yellow powder crystal. Figure 1 and 2 depict the unit cell and the primitive cell using brilloun zone sampling respectively.

II. Results and Discussion

2.1. Density Functional Theory

Density functional theory DFT [14] calculations to be done using LDA CAPZ functional for electronic properties of GaN with different electronic pseudopotentials. Also the pseudopotentials calculations done with different relativistic treatment. All the calculations were done for hexagonal GaN. The configuration of electrons in Ga is $[Ar]4s^2\ 3d^{10}4p^1$ and for N is $1s^2 2s^2 2p^3$. For all pseudopotentials, we have done the geometry optimisation considering different relativistic treatment. Then the energy band structure and state density measurement done for the variable pseudopotentials. All the pseudopotential for GaN has their own cut-off energy in the 5 ×5 ×4 K-points. In this work, we taken four pseudopotentials [15] i.e., OTFG ultrasoft, OTFG norm conserving, norm conserving [16], ultrasoft. There will be three relativistic treatments for each pseudopotential i.e., Schrodinger, Koelling Harman, Zora. Solutions to the atomic electronic structure and a pseudo atom involves in the calculations of OTFG(On the fly generation) pseudopotentials. For this calculations are done in Non relativistic (schroedinger) framework or using scalar relativistic approaches (Koelling-Harmon or Zora). In this work we calculated Band gap with different pseudopotentials (Table-1). We found that the OTFG ultrasoft pseudopotentials with Schroedinger relativistic treatment gives good results for GaN . For the Ultrasoft pseudopotential, the band gap found to be same 2.027 eV in all Schrodinger, Koelling Harman, Zora. For the norm conserving pseudopotential, the observed band gap must be same 1.971 eV in Schrodinger, Koelling Harman, Zora. In this work ,we find an interesting fact that for the Ultrasoft pseudopotential as well for the norm conserving pseudopotential ,the respective band gap is same irrespective of the relativistic treatment chosen. Energy density states and partial density of energy states plot draw and compared among pseudopotentials.

Figure-3 represents the band gap structure with different pseudopotentials. In the same symmetry line i.e., in gamma line, the conduction energy band minimum and

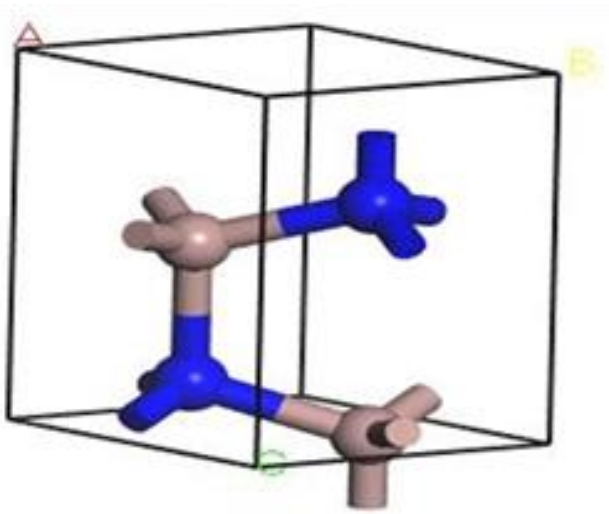

Fig. 1. Crystal structure of GaN Ga in grey and N in blue.

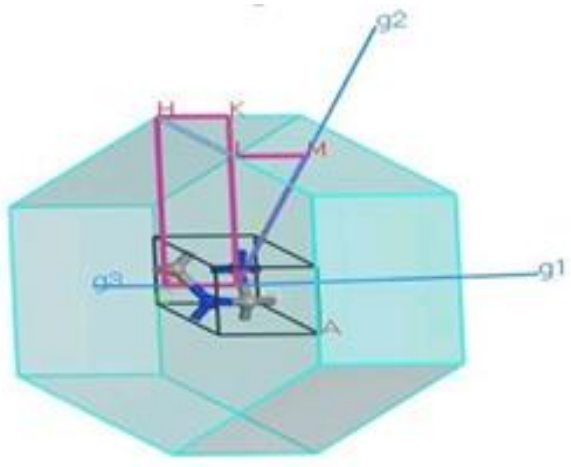

Fig. 2. Brillouine zone of GaN.

Table 1.

Band gap calculation of LDA CAPZ functional with different Pseudopotentials for GaN for 5 ×5 ×4 k-points

Pseudopotentials	Relativistic Treatment	Lattice constants after geometry optimization BFGS scheme[17](In Å)		Band gap (eV)
		a=b	c	
OTFG Ultrasoft (Cutoff Energy=517eV)	Schroedinger	3.16645	5.15480	2.202
	Koelling- Harmon	3.15631	5.14204	2.079
	Zora	3.15812	5.14491	2.069
OTFG norm conserving (Cutoff Energy=1116eV)	Schroedinger	3.17333	5.16808	2.147
	Koelling- Harmon	3.16401	5.15665	2.019
	Zora	3.16532	5.15760	2.014
Ultrasoft (Cutoff Energy=295eV)	Schroedinger	3.16546	5.15777	2.027
	Koelling- Harmon	3.16585	5.15769	2.027
	Zora	3.16551	5.15782	2.027
Norm conserving (Cutoff Energy=800eV)	Schroedinger	3.17789	5.17845	1.971
	Koelling- Harmon	3.17789	5.17845	1.971
	Zora	3.17789	5.17845	1.971

the valence-band maximum occurs. This concludes that the GaN is a direct energy bandgap semiconductor. With differing relativistic treatments, all pseudopotentials energy band shapes are essentially the same. The limitations of standard DFT calculations are what cause the band gap calculations to differ from the experimental result.

2.2. Local Density Approximation

In LDA, system's energy is represented as a function of electron density. It is a function of the coordinates of all electrons in the system. LDA functional was typically written in the following form:

$$E_{LDA} = \int \rho(\boldsymbol{r})\varepsilon xc[\rho(\boldsymbol{r})]\, d\boldsymbol{r}$$

where $E_{I,DA}$ was total energy of system, $\rho(\boldsymbol{r})$ was the position of electron density at r. $\varepsilon xc[\rho(\boldsymbol{r})$ was the exchange-correlation energy density. The energy density of exchange-correlation describes the interaction between electrons, taking into account the Pauli exclusion principle and the Coulomb interaction.

In LDA, the energy density of exchange-correlation is approximated as a function of the local electron density, which means that the functional depends only on electronic density at a given point in space and not on the density elsewhere in system. The LDA approximation assumes that the energy density of exchange-correlation at a point is determined by the local electron density, and that the electron density is smooth and continuous. While the LDA functional is relatively simple, it can provide useful predictions of the electronic properties of materials, and is still used in many DFT calculations today.

In quantum mechanical computations of materials, pseudopotentials are a frequently used method to lessen the computational work needed to solve the electronic structure problem. The explicit treatment of every electron in a system during a comprehensive ab-initio computation necessitates the employment of several basis functions to represent the electron wave functions. In particular, for bigger systems, this can make the computation highly computationally expensive. The complete potential that valence electrons in a solid experience is approximated by pseudopotentials. In order to create them, the core electrons from the full potential are removed. Their place is taken by an effective potential that accurately reproduces the valence electron wave functions. By ignoring the role of the core electrons, the resulting pseudopotential can be utilised to explain the valence electron states of a system. The two basic categories of pseudopotentials are:

- Norm-conserving pseudopotential
- Ultrasoft pseudopotential

Norm-conserving pseudopotentials are made to preserve the wave function's norm which guarantees that the system's overall charge is preserved. The number of basis functions needed to express the wave functions can be decreased by Ultrasoft pseudopotentials. This intended to be significantly smoother than norm-conserving pseudopotentials. The generation process is the primary distinction between On-The-Fly-Generated (OTFG) Ultrasoft and Norm-conserving pseudopotentials and conventional Ultrasoft and Norm-conserving pseudopotentials. OTFG pseudopotentials are formed on the fly during the calculation using a pre-set set of rules, in contrast to traditional pseudopotentials that are generated based on a set of predefined framework.

The Ultrasoft pseudopotential is defined as

$$\mathrm{V}(\mathbf{r}) = \sum_{\mathrm{G}\neq 0}[\mathrm{V}(\mathbf{G})\exp(-\mathrm{q}(\mathbf{G})^2\,\mathrm{r}^2)(1-\exp(-\mathrm{q}(\mathbf{R})^2\,\mathrm{r}^2))\,/\,\mathrm{q}(\mathbf{R})^2]$$

where V(**r**) is pseudopotential at position **r**. V(**G**) is Fourier transform of the potential. q(**G**) and q(R) are screening parameters.

The norm-conserving pseudopotential is defined as

$$\mathrm{V}(\mathbf{r}) = \sum_{\mathrm{G}\neq 0}[\mathrm{V}(\mathbf{G})\exp(\mathrm{i}\,\mathbf{G}\cdot\mathbf{r})]$$

where V(r) is the pseudopotential at position r. G is the

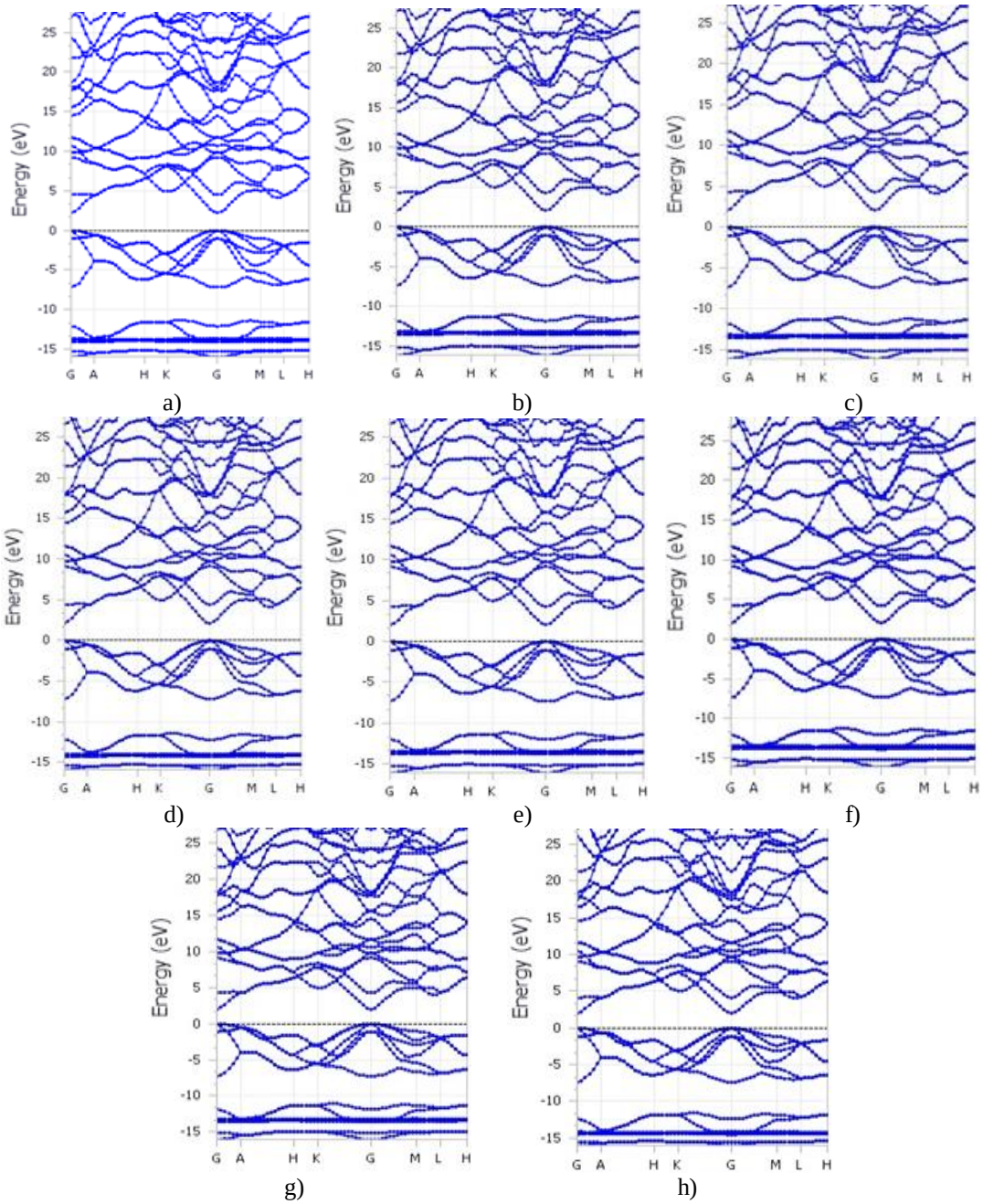

Fig. 3. Band gap calculation of LDA CAPZ functional with different Pseudopotentials for GaN for 5 ×5 ×4 k-points (a) OTFG Ultrasoft Schroedinger (b) OTFG Ultrasoft Koelling- Harmon (c) OTFG Ultrasoft Zora (d) OTFG norm conserving Schroedinger (e) OTFG norm conserving Koelling- Harmon (f) OTFG norm conserving Zora (g) ultrasoft Schroedinger / Koelling- Harmon/ Zora (h) norm conserving Schroedinger / Koelling- Harmon / Zora (Table – 1).

reciprocal lattice vector. OTFG pseudopotentials more efficient and accurate than traditional pseudopotentials, but it requires more computational resources to generate.

Figure-4 represents the total energy density states (DOS) of GaN of different pseudopotentials. The behaviour of non-relativistic particles is described by the Schroedinger equation, a key equation in quantum mechanics [18-20]. Relativistic treatments of pseudopotentials frequently utilised in solid state physics include Koelling Harmon and Zora. While Zora is a fully relativistic method that accounts for both the effects of relativity and the mobility of atomic nuclei. Koelling Harmon is a semi-relativistic approach that approximates the valence electrons of an atom as linear combination of atomic like wave functions [21-23]. While Koelling Harmon is a fair balance between accuracy and computing economy for some materials. Zora is thought to be the most precise technique for handling relativistic effects but is computationally expensive. [24-27].

In all diagrams, Fermi energy is assumed to be Zero of the energy axis. On left and right sides of fermi energy line, there are valence and conduction band respectively. More electrons in the valence band indicates that GaN is a semiconducting material. Two frequently utilised approximations in density functional theory simulations for forecasting the electrical characteristics of materials are LDA and GGA. Compared to more sophisticated approaches, both of these approximations offer a more

straightforward and computationally effective means of characterising the electron density of a material. Energy difference between the LUMO and HOMO is known as band gap in DFT calculations.

One explanation is that the LDA and GGA methods are predicted on the idea that a material's electron density is homogeneous and does not appreciably change with position. For some material's, especially those with intricate crystal structures or strong electrical correlations, this presumption might not be accurate. As a result of failing to completely take into consideration the localised character of electrons, LDA and GGA approaches may overestimate the band gap. Another factor is that the exact exchange correlation potential, a key factor in DFT calculations, is not taken into consideration by the LDA and GGA approaches. It is challenging to calculate the precise exchange correlation potential; thus it is typically estimated using a variety of techniques. The band gap may be underestimated in LDA and GGA approaches because the approximations utilised do not completely account for

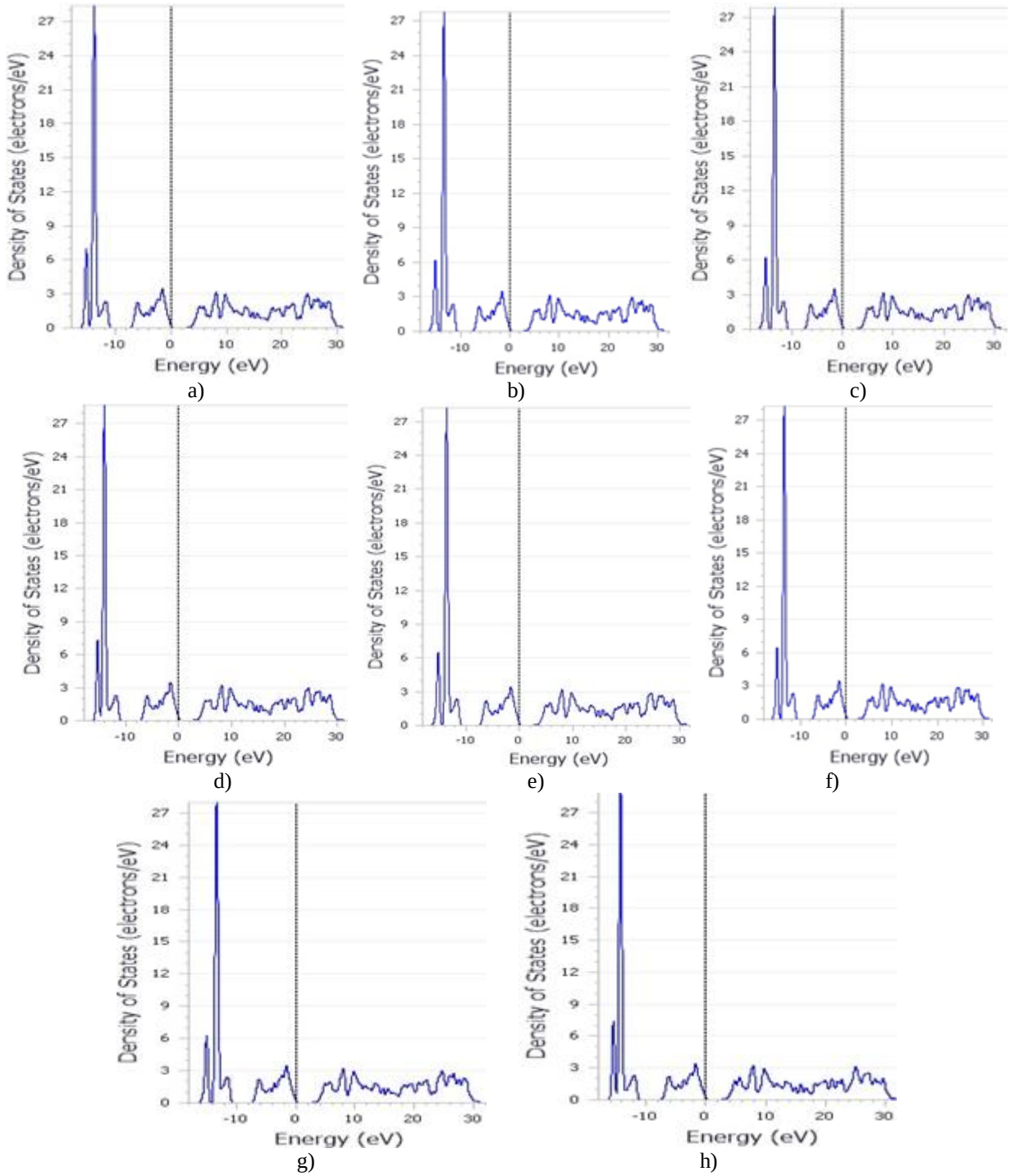

Fig. 4. Density of states calculation of LDA CAPZ functional with different Pseudopotentials for GaN for 5 ×5 ×4 k-points (a) OTFG Ultrasoft Schroedinger (b) OTFG Ultrasoft Koelling- Harmon (c) OTFG Ultrasoft Zora (d) OTFG norm conserving Schroedinger (e) OTFG norm conserving Koelling- Harmon (f) OTFG norm conserving Zora (g) ultrasoft Schroedinger / Koelling- Harmon/ Zora (h) norm conserving Schroedinger / Koelling- Harmon / Zora.

the exchange correlation effects. Due to the simplifications and assumptions utilised in these method, especially for materials with complicated electrical characteristics, energy band-gap predicted by LDA and GGA methods may vary less than real value.

Figure-5 represents the partial energy density of states of GaN of different pseudopotentials. Contribution of electrons from different orbitals can clearly

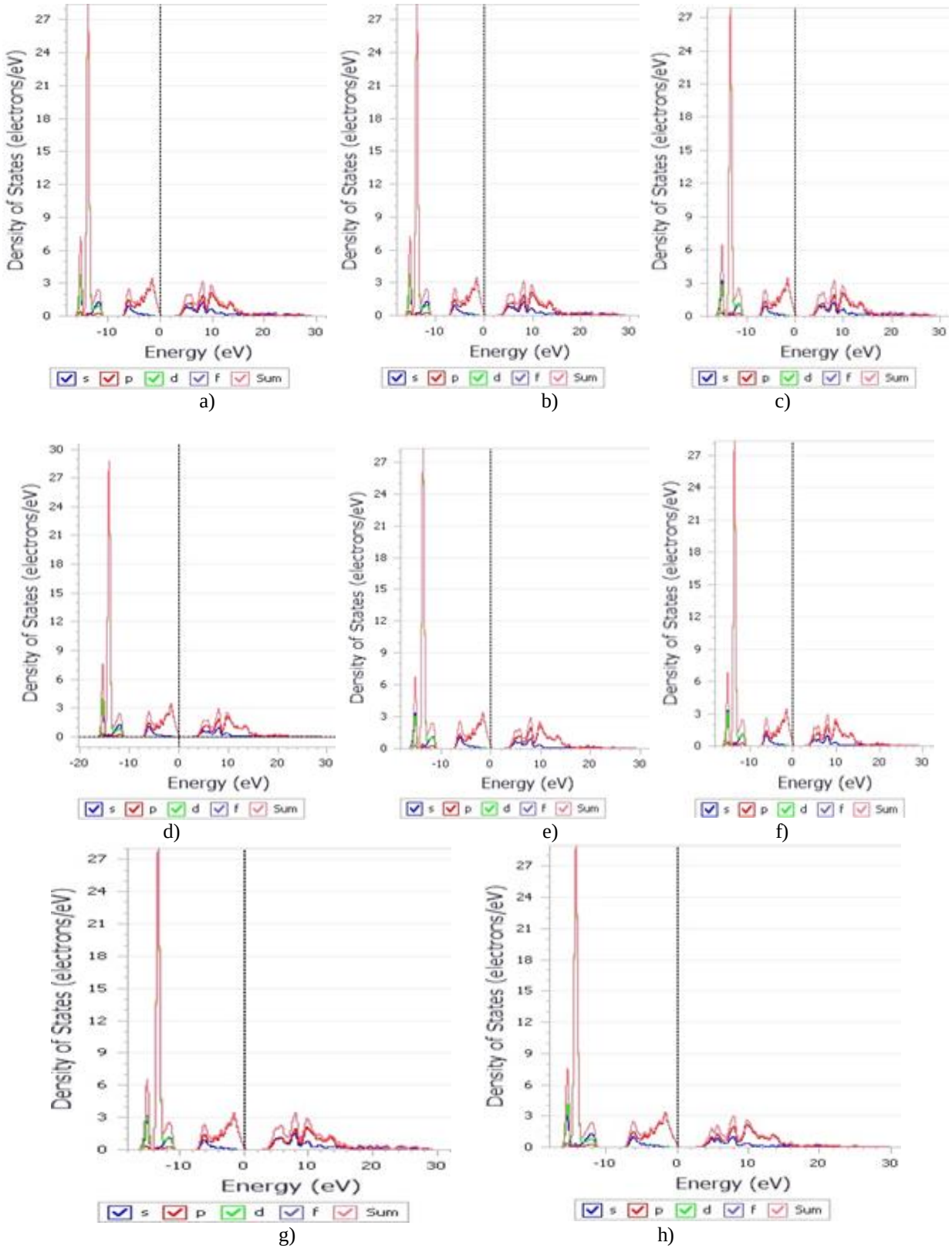

Fig. 5. Partial Energy Density of states calculation of LDA CAPZ functional with different Pseudopotentials for GaN for 5 ×5 ×4 k-points (a) OTFG Ultrasoft Schroedinger (b) OTFG Ultrasoft Koelling- Harmon (c) OTFG Ultrasoft Zora (d) OTFG norm conserving Schroedinger (e) OTFG norm conserving Koelling- Harmon (f) OTFG norm conserving Zora (g) ultrasoft Schroedinger/Koelling- Harmon/Zora (h) norm conserving Schroedinger/Zoralling- Harmon / zora.

understandable from PDOS plot. The p-state electrons contribute more in both valence and conduction band. The d-state electrons present inner portion to valence band.

Conclusions

The structural and electronic properties calculations are done with first-principle Density functional theory for GaN. The Band gaps were calculated using LDA CAPZ functional with different electronic pseudopotentials having different relativistic treatment for GaN. Also different cut-off energies are used in this observation. Energy density states and partial of energy density states were compared for all the pseudopotentials with different relativistic calculations. OTFG Ultrasoft pseudopotentials with Schroedinger relativistic treatment gave good results slightly less than compared to experimental results. The band gap found to be slightly different for different pseudopotentials. Distributions of valence electronic band's electronic states and conduction electronic band's electronic states are found to be same in GaN. Partial density of states plot gives good idea about the orbital contribution of electrons to the density of levels. The ultrasoft pseudopotential as well for the norm conserving pseudopotential, the respective band gap is same irrespective of the relativistic treatment chosen.

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Д. Кумар Дас, П. Патнайк, С. Кумар Наяк, М. Барала

Оцінка впливу електронних псевдопотенціалів і релятивістських процедур на структурні та електричні властивості GaN: дослідження методом функціоналу густини

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Застосовуючи принцип теорії функціоналу густини, можна обчислити різні параметри для GaN, такі як постійна гратки, ширина забороненої зони, зонна структура, поведінку діелектричної функції, показника заломлення, провідності, щільності станів, функцію втрат тощо. У цій роботі використано різні електронні псевдопотенціали із різною релятивістською обробкою, дослідженою за допомогою функціоналу апроксимації локальної густини (LDA-CAPZ) у DFT для GaN. Для розрахунку значень енергії використано зміни параметрів гратки після оптимізації геометрії та побудови зонних енергій. Результати розрахунків електронної структури є порівняннями різних електронних псевдопотенціалів з різною енергією відсічення із використанням різних релятивістських підходів. Графіки щільності та часткової щільності станів допомагають більше дізнатися про електронні та магнітні характеристики зразка. Крім того, виконано порівняння переваг та недоліків різних псевдопотенціалів з різними релятивістськими підходами для вибірки. Розподіл енергетичних рівнів і часткову щільність станів порівнювали для всіх псевдопотенціалів з різними релятивістськими обробками, що дало розуміння орбітальних внесків електронів у щільність станів. Дане дослідження забезпечує глибше розуміння впливу електронних псевдопотенціалів і релятивістських доданків на електронні та структурні властивості GaN.

Клбчові слова: DFT, LDA, псевдопотенціали, релятивістські трактування.