Comparative Analysis of Nitrides Band Structures Calculated by the Empirical Pseudopotential Method

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Abstract The electronic band structures of zinc blende and wurtzite GaN and InN are calculated using the empirical pseudopotential method, with the form factors adjusted to reproduce correctly the most important band features. To this end, a comprehensive analysis and comparison with several experimental and theoretical data reported in the literature is performed. Relevant energy spacings as well as direct and indirect band gaps are then derived from the band structures. The electron effective masses at high symmetry points are also obtained using a parabolic line fit. The calculated parameters are reported together with existing data so that they can be easily compared and used in the interpretation of experiments and for numerical simulation purposes.

Keywords Nitrides, Band structure, Pseudopotential empirical method

1 Introduction

In recent years, the interest in III-V nitrides has been increasing considerably because of their important technological applications due to their interesting electrical and optical properties. In particular, they have been widely investigated and exploited in the development of optoelectronic devices in the blue and ultraviolet spectral regions as well as for high power and high temperature electronics [1, 2, 3, 4, 5, 6, 7, 8]. An additional feature further enhances the III-V nitrides potential over other semiconductors: the strong interaction between the electrons and optical phonons [9, 10], a crucial property for the development of terahertz devices. In this context, it is very important to have access to all the information about the band structure details and transport parameters that are necessary in both experimen-

tal applications (device design and optimization), and theoretical modelling (Monte Carlo simulations, hydrodynamic calculations, etc.) [11].

Binary nitrides such as GaN, AlN and InN usually crystallize in the wurtzite structure, but can also be grown in the zinc blende structure [12, 13, 14]. Early studies of the interband optical absorption performed on InN thin films were interpreted as being consistent with a fundamental energy gap of about 2 eV [15, 16, 17, 18, 19]. Since 2002, improvements in epitaxial growth techniques enabled the availability of both wurtzite and zinc blende InN films of much higher quality with considerably low electron concentrations, much higher electron mobilities, but also lower oxygen defects caused by annealing in an oxygen atmosphere that leads to formation of InN-InO₂ alloys. Characterization of the obtained high-quality InN layers revealed for InN a band gap lower than 1 eV [20, 21, 22], much smaller than the previously reported values. Parallel to the experimental improvements, theoretical band structure calculations of wurtzite and zinc blende InN are being revised in order to fit experimental results [23, 24]. In this context, we present a theoretical investigation of the zinc blende and wurtzite band structures using an empirical pseudopotential approach (EPM), while providing sets of adjusted symmetrical and antisymmetrical pseudopotential form factors for InN consistently with those latest experimental results, but also for GaN and AlN whose band structures are also calculated for both zinc blende and wurtzite structures, in order to further validate our calculations. This will help the understanding of nitrides electronic properties and their important band structure parameters such as direct and indirect band gaps, effective masses and nonparabolicity coefficients.

The paper is organized as follows. The EPM is described in details for the zinc blende and wurtzite structures in Sections 2 and 3 respectively, in addition to the calculation of the nitrides band structures and derivation of the main energy spacings and effective masses. Sec-

tion 4 summarizes the results, while presenting a comparative analysis of the main III-nitrides parameters.

2 Band structure of zinc blende nitrides

2.1 Zinc blende structure

Let consider in the left panel of Fig. 1 the face-centered cubic lattice whose base vectors are given by: $\mathbf{a}_1 = (0, a/2, a/2)$, $\mathbf{a}_2 = (a/2, 0, a/2)$, and $\mathbf{a}_3 = (a/2, a/2, 0)$, where a is the side of the lattice [25]. The zinc blende structure is formed from this face-centered cubic lattice by placing at each site of the lattice an elementary pattern composed of an atom of zinc and an atom of sulphur separated by a distance equal to one quarter of the diagonal of the unit cell (see Fig. 1).

Figure 1. Face-centered cubic structure (left) and zinc blende lattice (right).

The reciprocal lattice of a face-centered cubic lattice, and as a consequence for a zinc blende structure, is a centered cubic lattice whose base vectors are given by [25]: $\mathbf{b}_1 = (2\pi/a)(-1, 1, 1)$, $\mathbf{b}_2 = (2\pi/a)(1, -1, 1)$, and $\mathbf{b}_3 = (2\pi/a)(1, 1, -1)$. Given the high symmetry of the Brillouin zone, the band structure calculations can be considerably reduced using the symmetry operations of the crystal. It can be easily proved that a reduced region representing $1/48^{th}$ of the Brillouin zone is sufficient to determine the energetic structure of the zinc blende crystals [25]. The reduced region is delimited by the following points whose coordinates are given in units of $(2\pi/a)$: $\Gamma = (0, 0, 0)$, $X = (0, 1, 0)$, $K = (0.75, 0.75, 0)$, $L = (0.5, 0.5, 0.5)$, and $U = (0.25, 1, 0.25)$ (see left panel of Fig. 2).

Figure 2. Brillouin zones of the zinc blende (left) and wurtzite (right) structures.

2.2 Semi-empirical pseudopotential calculation for zinc blende nitrides

The one-electron Schrödinger equation resulting from the variational method by using a base of plane waves is [26]:

$$\left[\frac{\hbar^2}{2m} (\mathbf{k} + \mathbf{g})^2 - \epsilon \right] C_{\mathbf{k}+\mathbf{g}} + \sum_{\mathbf{g}'} V_{\mathbf{g}-\mathbf{g}'} C_{\mathbf{k}+\mathbf{g}'} = 0 \quad (1)$$

where $\mathbf{k}$ is a vector of the first Brillouin zone, $\mathbf{g}$ a vector of the reciprocal lattice, ϵ the energy eigenvalues, $V_{\mathbf{g}-\mathbf{g}'}$ ($V_{\Delta\mathbf{g}}$) the pseudopotential and C the eigenvector of the Hamiltonian.

We notice that (1) can be reduced to the form $HC = \epsilon C$, where the elements of the matrix H can be written as:

$$H_{\mathbf{g},\mathbf{g}'} = \left(\frac{\hbar^2}{2m} |\mathbf{k} + \mathbf{g}|^2 \delta_{\mathbf{g},\mathbf{g}'} + V_{\mathbf{g},\mathbf{g}'} \right) \quad (2)$$

In this expression, $V_{\mathbf{g},\mathbf{g}'} = V_{\Delta\mathbf{g}} = \sum V_r \exp(-i\Delta\mathbf{g} \cdot \mathbf{r})$, where the sum is over the atoms of the unit cell. We consider the origin at the midpoint between the two atoms of the unit cell so that $\mathbf{r}_a = (\frac{a}{8})(1, 1, 1) = \mathbf{s}$ and $\mathbf{r}_b = (-\frac{a}{8})(1, 1, 1) = -\mathbf{s}$ (see left panel of figure 3).

$$V_{\Delta\mathbf{g}} = V_{\Delta\mathbf{g}}^s \cos\left[\left(\frac{\pi}{4}\right)(\Delta g_x + \Delta g_y + \Delta g_z)\right] - iV_{\Delta\mathbf{g}}^a \sin\left[\left(\frac{\pi}{4}\right)(\Delta g_x + \Delta g_y + \Delta g_z)\right] \quad (3)$$

where $V_{\Delta\mathbf{g}}^s$ and $V_{\Delta\mathbf{g}}^a$ are the symmetrical and anti-symmetrical pseudopotential form factors respectively. They are treated as adjustable parameters that can be adapted with experimental data, which explains why the method is called *semi-empirical* pseudopotential method [26]. In other terms, the band structure calculations are made using experimental data that are adjusted until the results of the calculations agree with the experience.

Figure 3. Elementary patterns of the zinc blende (left) and wurtzite (right) structures.

A vector $\mathbf{g} = l\mathbf{b}_1 + m\mathbf{b}_2 + n\mathbf{b}_3$ of the reciprocal lattice can be expressed as:

$$\mathbf{g} = \left(\frac{2\pi}{a}\right)[(-l+m+n)\mathbf{a}_1 + (l-m+n)\mathbf{a}_2 + (l+m-n)\mathbf{a}_3] \quad (4)$$

Its norm is then given by:

$$|\mathbf{g}|^2 = \left(\frac{2\pi}{a}\right)^2 (3l^2 + 3m^2 + 3n^2 - 2lm - 2mn - 2ln) \quad (5)$$

Therefore, the groups of vectors of the zinc blende structure are (coordinates are in units of $2\pi/a$):

- $\mathbf{g}_0 \equiv (0, 0, 0)$ (the origin)

Table 1. Pseudopotential form factors (in Ry) of zinc blende GaN, AlN and InN used in the calculations.

	V_3^s	V_8^s	V_{11}^s	V_3^a	V_4^a	V_{11}^a
GaN	-0.2218	0.0180	0.0989	0.3360	0.2430	0.0400
AlN	-0.3284	-0.0374	0.2341	0.2311	0.2757	-0.0101
InN	-0.2186	-0.0055	0.0569	0.0811	0.0531	0.0314

Table 2. Eigenenergies of zinc blende GaN, AlN and InN for the high-symmetry points Γ , X and L . The values are in eV and are given with respect to Γ_{15}^v . Our calculations are evidenced by the asterisk, while all other values have been taken from the literature.

	GaN	AlN	InN
Γ_{15}^v	0.00*, 0 ^[27] , 0.0(0.0) ^[28] , 0.000 ^[18, 29, 30]	0.00*, 0 ^[27] , 0.000 ^[18, 29] , 0.0(0.0) ^[28]	0.00*, 0.0 ^[24] , 0.000 ^[23, 31]
Γ_1^c	3.23*, 3.20 ^[27] , 2.1(3.1) ^[28] , 3.1 ^[32] , 3.200 ^[33] , 3.308 ^[18] , 3.383 ^[29] , 3.213 ^[30]	5.88*, 5.91 ^[27] , 5.914 ^[33] , 6.0 ^[32] , 5.840 ^[18] , 5.936 ^[29] , 4.2(6.0) ^[28]	0.51*, 0.592 ^[23] , 0.435 ^[31]
Γ_{15}^c	12.11*, 12.14 ^[27] , 10.098 ^[18] , 10.300 ^[29] , 10.248 ^[30] , 10.6(12.2) ^[28]	13.99*, 14.16 ^[27] , 12.579 ^[18] , 13.406 ^[29] , 12.3(14.6) ^[28]	9.08*, 9.597 ^[23] , 10.174 ^[31]
X_3^v	-5.45*, -5.47 ^[27] , -6.294 ^[18] , -6.149 ^[29] , -5.923 ^[30] , -6.5(-6.9) ^[28]	-5.19*, -5.26 ^[27] , -5.388 ^[18] , -5.262 ^[29] , -5.0(-5.6) ^[28]	-5.41*, -5.5 ^[24] , -4.795 ^[23] , -4.687 ^[31]
X_5^v	-2.28*, -2.29 ^[27] , -2.459 ^[18] , -2.693 ^[29] , -2.086 ^[30] , -2.8(-3.0) ^[28]	-1.92*, -1.98 ^[27] , -2.315 ^[18] , -2.337 ^[29] , -1.8(-2.1) ^[28]	-2.25*, -2.8 ^[24] , -1.481 ^[23] , -1.687 ^[31]
X_1^c	4.72*, 4.70 ^[27] , 4.428 ^[18] , 4.571 ^[29] , 4.585 ^[30] , 4.7 ^[32] , 4.700 ^[33] , 3.2(4.7) ^[28]	4.91*, 4.92 ^[27] , 4.918 ^[33] , 4.9 ^[32] , 5.346 ^[18] , 5.102 ^[29] , 3.2(4.9) ^[28]	4.38*, 4.758 ^[23] , 2.903 ^[31]
X_3^c	7.45*, 7.46 ^[27] , 6.010 ^[18] , 6.805 ^[29] , 6.265 ^[30] , 12.2(14.5) ^[28]	10.07*, 10.10 ^[27] , 8.794 ^[18] , 10.661 ^[29] , 14.1(17.3) ^[28]	5.78*, 5.102 ^[23] , 6.322 ^[31]
L_1^v	-6.15*, -6.19 ^[27] , -6.812 ^[18] , -6.743 ^[29] , -6.644 ^[30] , -7.4(-7.8) ^[28]	-5.86*, -5.98 ^[27] , -6.251 ^[18] , -6.179 ^[29] , -6.0(-6.7) ^[28]	-6.51*, -6.5 ^[24] , -4.967 ^[23] , -5.229 ^[31]
L_3^v	-0.74*, -0.78 ^[27] , -0.834 ^[18] , -0.931 ^[29] , -0.772 ^[30] , -1.0(-1.1) ^[28]	-0.68*, -0.75 ^[27] , -0.718 ^[18] , -0.728 ^[29] , -0.5(-0.6) ^[28]	-0.69*, -1.0 ^[24] , -0.460 ^[23] , -0.557 ^[31]
L_1^c	6.23*, 6.20 ^[27, 32] , 6.200 ^[33] , 5.149 ^[18] , 5.636 ^[29] , 5.510 ^[30] , 5.0(6.2) ^[28]	9.14*, 9.08 ^[27] , 9.079 ^[33] , 9.3 ^[32] , 8.264 ^[18] , 9.423 ^[29] , 10.0(12.6) ^[28]	4.39*, 3.213 ^[23] , 3.813 ^[31]
L_3^c	11.22*, 11.19 ^[27] , 10.416 ^[18] , 9.916 ^[29] , 10.606 ^[30] , 10.6(12.3) ^[28]	11.85*, 11.91 ^[27] , 12.202 ^[18] , 12.014 ^[29] , 11.0(13.2) ^[28]	7.52*, 10.040 ^[23] , 6.954 ^[31]

Table 3. Energy gaps of zinc blende GaN, AlN and InN for the high-symmetry points Γ , X and L . Our calculations are evidenced by the asterisk, while all other values have been taken from the literature. All values are in eV.

	GaN	AlN	InN
$E_g^{\Gamma-\Gamma}$	3.23*, 3.20 ^[27, 34] , 3.10 ^[35, 28] , 3.21 ^[30] , 3.38 ^[29, 36] , 3.17 ^[15] , 3.82 ^[37] , 3.26 ^[38] , 3.25 ^[39] , 3.43 ^[40] , 3.2 ^[41] , 3.299 ^[42] , 2.08 ^[43] , 2.65 ^[44]	5.88*, 6.0 ^[28, 41, 42, 45] , 5.914 ^[27] , 6.02 ^[15] , 5.94 ^[29] , 6.27 ^[37] , 6.18 ^[40] , 6.20 ^[36]	0.51*, 0.592 ^[23] , 0.435 ^[31]
$E_g^{\Gamma-X}$	4.72*, 4.70 ^[27, 28, 35] , 4.58 ^[30] , 4.57 ^[29, 40, 36] , 4.61 ^[37] , 4.7 ^[41] , 4.52 ^[42]	4.91*, 4.9 ^[28, 41, 42, 45] , 4.918 ^[27] , 4.92 ^[15] , 5.10 ^[29, 40, 36] , 5.24 ^[37]	4.38*, 4.758 ^[23] , 2.903 ^[31]
$E_g^{\Gamma-L}$	6.23*, 6.20 ^[27, 28, 35] , 5.51 ^[30] , 5.64 ^[29, 36] , 5.97 ^[37] , 5.66 ^[40] , 6.2 ^[41] , 5.59 ^[42]	9.14*, 9.079 ^[27] , 9.3 ^[28, 41, 42] , 9.70 ^[37] , 9.42 ^[29, 36] , 9.43 ^[40] , 9.21 ^[45]	4.39*, 3.213 ^[23] , 3.831 ^[31]
E_g^{L-L}	6.97*, 6.9 ^[38] , 7.0 ^[46]	9.82*	5.08*, 3.673 ^[23] , 3.85 ^[31]
E_g^{X-X}	7.00*, 7.2 ^[38] , 7.6 ^[46]	6.83*	6.63*, 6.239 ^[23] , 4.59 ^[31]

Table 4. Effective masses of zinc blende GaN, AlN and InN. Our calculations are evidenced by the asterisk, while all other values have been taken from the literature. All values are in units of the free electron mass.

	GaN	AlN	InN
m_e	0.1393*, 0.12 ^[30] , 0.11 ^[15] , 0.13 ^[29] , 0.15 ^[47] , 0.14 ^[38] , 0.21 ^[48] , 0.124 ^[49] , 0.127 ^[41] , (0.15 ± 0.01) ^[39]	0.271*, 0.23 ^[18] , 0.28 ^[50] , 0.21 ^[29, 45, 47] , 0.19 ^[15] , 0.209 ^[41] , 0.30 ^[51] , 0.25 ^[39, 42]	0.1140*, 0.066 ^[23] , 0.07 ^[52]
$m_{hh}^{[100]}$	0.9807*, 0.84 ^[18] , 0.86 ^[50] , 0.76 ^[53] , 0.85 ^[51] , 0.85 ^[42] , 1.34 ^[30]	1.3114*, 1.02 ^[18] , 1.44 ^[50] , 1.05 ^[53] , 1.39 ^[51] , 1.02 ^[42]	0.8381*, 1.262 ^[23] , 0.83 ^[52]
$m_{lh}^{[100]}$	0.1624*, 0.22 ^[18] , 0.21 ^[50] , 0.21 ^[53] , 0.24 ^[51] , 0.24 ^[42] , 0.70 ^[30]	0.2925*, 0.37 ^[18] , 0.42 ^[50] , 0.35 ^[53] , 0.44 ^[51] , 0.35 ^[42]	0.0984*, 0.100 ^[23] , 0.16 ^[52]
$m_{hh}^{[111]}$	2.6063*, 2.07 ^[18] , 2.09 ^[50] , 1.93 ^[53] , 1.79 ^[51] , 2.13 ^[42] , 1.06 ^[30]	3.0688*, 2.64 ^[18] , 4.24 ^[50] , 2.73 ^[53] , 3.85 ^[51] , 4.55 ^[42]	2.2593*, 2.744 ^[23] , 0.83 ^[52]
$m_{lh}^{[111]}$	0.1350*, 0.19 ^[18] , 0.19 ^[50] , 0.18 ^[53] , 0.21 ^[51] , 0.21 ^[42] , 0.63 ^[30]	0.2343*, 0.30 ^[18] , 0.36 ^[50] , 0.30 ^[53] , 0.36 ^[51] , 0.28 ^[42]	0.0859*, 0.096 ^[23] , 0.16 ^[52]
$m_{hh}^{[110]}$	0.9763*, 1.52 ^[18] , 1.65 ^[50] , 1.51 ^[53] , 1.40 ^[51] , 1.55 ^[42] , 1.44 ^[30]	1.3140*, 1.89 ^[18] , 3.03 ^[50] , 2.16 ^[53] , 2.67 ^[51] , 2.44 ^[42]	0.8397*, 2.122 ^[23] , 1.55 ^[52]
$m_{lh}^{[110]}$	0.1412*, 0.20 ^[18] , 0.19 ^[50] , 0.19 ^[53] , 0.21 ^[51] , 0.21 ^[42] , 0.58 ^[30]	0.2468*, 0.32 ^[18] , 0.37 ^[50] , 0.31 ^[53] , 0.38 ^[51] , 0.29 ^[42]	0.0887*, 0.097 ^[23] , 0.15 ^[52]

- $\mathbf{g}_3 \equiv (-1, -1, -1), (\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1), (1, 1, 1)$
- $\mathbf{g}_4 \equiv (-1, -1, 0), (-1, 0, -1), (0, -1, -1), (0, 1, 1), (1, 0, 1), (1, 1, 0)$
- $\mathbf{g}_8 \equiv (-2, -1, -1), (-1, -2, -1), (-1, -1, -2), (-1, 0, 1), (-1, 1, 0), (0, -1, 1), (0, 1, -1), (1, -1, 0), (1, 0, -1), (1, 1, 2), (1, 2, 1), (2, 1, 1)$
- $\mathbf{g}_{11} \equiv (-2, -2, -1), (-2, -1, -2), (-2, -1, 0), (-2, 0, -1), (-1, -2, -2), (-1, -2, 0), (-1, -1, 1), (-1, 0, -2), (-1, 1, -1), (-1, 1, 1), (0, -2, -1), (0, -1, -2), (0, 1, 2), (0, 2, 1), (1, -1, -1), (1, -1, 1), (1, 0, 2), (1, 1, -1), (1, 2, 0), (1, 2, 2), (2, 0, 1), (2, 1, 0), (2, 1, 2), (2, 2, 1)$
- $\mathbf{g}_{12} \equiv (-2, -2, -2), (\pm 2, 0, 0), (0, \pm 2, 0), (0, 0, \pm 2), (2, 2, 2) \dots$

Figure 4. Band structure of zinc blende GaN obtained by our pseudopotential calculations.

Actually, only 4 groups of vectors are practically necessary for the calculations [26]. As a matter of fact, the form factor V_0 corresponding to $\mathbf{g}_0$ is a constant potential that shifts the whole energetic scale of a quantity V_0 . This is the reason why we can attribute to V_0 the

Figure 5. Band structure of zinc blende AlN obtained by our pseudopotential calculations.

value zero or any other adequate value. Besides, we can neglect the pseudopotential form factors corresponding to $g^2 > 11(2\pi/a)^2$, because V_g typically decreases as $1/g^2$ for high values of g [26]. Furthermore, the symmetrical term corresponding to $\mathbf{g}_4$ and the antisymmetrical term corresponding to $\mathbf{g}_8$ are always null because $\cos(\mathbf{g}_4 \cdot \mathbf{s}) = \sin(\mathbf{g}_8 \cdot \mathbf{s}) = 0$ for any $\mathbf{g}_4$ or $\mathbf{g}_8$ vector. Therefore, only 6 pseudopotential form factors are sufficient for the calculation: $V_3^s, V_8^s, V_{11}^s, V_3^a, V_4^s$ and V_{11}^a .

In Table 1 are given the pseudopotential form factors of the zinc blende GaN and InN that we recommend and that we used in our calculations. In particular, the pseudopotential form factors of InN have been adapted to reproduce a band structure in good agreement with the latest experimental results. The lattice constants used for zinc blende GaN, AlN and InN are: 0.44953 nm [27], 0.43752 nm [27] and 0.4986 nm [54, 55] respectively.

We still have to choose the size of the Hamiltonian matrix whose diagonal elements are given by:

$$H_{i,i} = \left(\frac{\hbar^2}{2m} \right) |\mathbf{k} + \mathbf{g}_i|^2, \quad (6)$$

and non-diagonal elements are given by:

$$H_{i,j} = V_s(|\mathbf{g}_i - \mathbf{g}_j|) \cos[(\mathbf{g}_i - \mathbf{g}_j) \cdot \mathbf{s}] + iV_a(|\mathbf{g}_i - \mathbf{g}_j|) \sin[(\mathbf{g}_i - \mathbf{g}_j) \cdot \mathbf{s}] \quad (7)$$

for $i \neq j$.

It is evident that the size of the Hamiltonian matrix depends on the chosen number of reciprocal lattice vectors. For that purpose, we choose a maximum value to limit the norm of the chosen reciprocal vectors given by (5). In our case, we have verified that the condition $|\mathbf{g}|^2 < 21(2\pi/a)^2$ (corresponding to a set of 113 reciprocal vectors) provides sufficiently accurate results. In this way, we can calculate all the elements of the Hamiltonian matrix using (6) and (7). The diagonalization of the Hamiltonian matrix gives directly the eigenvalues of the electronic states corresponding to the vector $\mathbf{k}$ of the Brillouin zone.

2.3 Results

The energetic band structures obtained by our pseudopotential calculations are represented in figures 4, 5 and 6 for zinc blende GaN, AlN and InN respectively, along the high-symmetry points Γ , X , U , L , and K of the Brillouin zone. We notice that the energy reference level matches the top of the valence band. From a qualitative point of view, the overall shape of the valence and conduction bands that we have obtained for zinc blende GaN and AlN is similar to that obtained by Fritsch *et al.* [18], Al-Douri *et al.* [37], Pugh *et al.* [15] and Aourag *et al.* [27, 33]. The same occurs for zinc blende InN whose overall shape of the valence and conduction bands is similar to the reexamined band structures of Fritsch *et al.* [23] and King *et al.* [24].

Figure 6. Band structure of zinc blende InN obtained by our pseudopotential calculations.

In order to quantitatively compare the obtained band structures with other results, the obtained energetic eigenvalues are given in Table 2 for the high-symmetry points Γ , X and L . All eigenvalues are given with respect to the top of the valence band Γ_{15}^v . We note first that all results and calculations before 2002 that do not take into consideration the new corrections brought into the band structure of InN have not been included in our comparison. In addition, we note that the values corresponding to ref. [24] are approximate values that we

have estimated from the band structure of zinc blende InN obtained by King *et al.* [24], since no accurate values are available in the article, but only the obtained band structure. On the other hand, in ref. [28], there are two values proposed for each energetic eigenvalue, both calculated by the local-density approximation (LDA), but the value in parenthesis is the result of an additional correction by the Green's function approximation (GW) which takes into consideration the Coulomb screening effect of the electrons [28]. We can initially point out the zero value assigned to Γ_{15}^v by all cited references [27], [33], [32], [28], [18], [23], [29], and [30], which means that the energy reference level has been taken at the top of the valence band in all calculations. Regarding the results of zinc blende GaN and AlN, we remark an excellent agreement between our results and those found by Aourag *et al.* [27, 33] since the relative difference between the results does not exceed 2% for most of the energy eigenvalues, and even 0.5% for some of them.

We also observe a general agreement with the results of references [18], [29], [30] and [32] and ours, since their relative deviation does not exceed 10% for most energy eigenvalues. As for the calculations performed by Rubio *et al.* [28], there's a good agreement with our results for the eigenenergies Γ_{15}^v , Γ_1^v , Γ_{15}^c , X_5^v , X_1^c , and L_3^c corresponding to GaN and AlN, for L_1^c corresponding to GaN, and for X_3^v and L_3^v corresponding to AlN. But the eigenvalues Γ_1^v , X_1^v , X_3^c of GaN and AlN are widely overestimated (by at least 20%) in [28]. We also notice an underestimation of the eigenvalues X_3^v and L_3^v corresponding to GaN with respect to our results and to other calculations. On the other hand, regarding the results of zinc blende InN, we first remark a slight underestimation of most valence band eigenenergies obtained by our calculations with respect to those of references [23] and [31]. This is due to the fact that we have adapted our valence band structure to the very recent results by King *et al.* obtained by a combination of experimental characterization by high-resolution x-ray photoemission spectroscopy assisted by theoretical calculations via the quasiparticle corrected density functional theory [24]. Despite this slight underestimation, our values are generally in good agreement with the results of the cited works of Fritsch *et al.* [23], Bechstedt *et al.* [31] and of course King *et al.* [24].

In order to ensure the precision of our semi-empirical results in comparison to other semi-empirical and *ab-initio* calculations and experimental results, the values of the bandgaps $E_g^{\Gamma-\Gamma}$, $E_g^{\Gamma-X}$, $E_g^{\Gamma-L}$, E_g^{X-X} and E_g^{L-L} at high-symmetry points Γ , X and L are shown in Table 3. Regarding the energy spacings of GaN and AlN, we remark a good agreement between the values found by our calculations and those of most other references in Table 3. Even the bandgap values given by Rubio *et al.* [28] agree with our calculations. As a matter of fact, for most values of Table 3, the relative difference between our calculations and those of the other references does not exceed 10%. Only the values of $E_g^{\Gamma-\Gamma}$ proposed by Al-Douri *et al.* [37] and Palummo *et al.* [44] for zinc blende GaN make an exception: Palummo underestimates the gap value to 2.65 eV and Al-Douri overestimates it to 3.82 eV. However, the value of $E_g^{\Gamma-\Gamma}$ for AlN and the values of $E_g^{\Gamma-X}$ and $E_g^{\Gamma-L}$ for GaN and

AlN proposed by Al-Douri *et al.* are in good agreement with our calculations. The slight disagreements do not prevent a general good agreement with other theoretical and experimental results. As for the obtained energy spacings for zinc blende InN, they are in good agreement with the results of Fritsch *et al.* [23] and Bechstedt *et al.* [31], despite the slight overestimation of the energy spacings $E_g^{\Gamma-L}$, E_g^{L-L} and E_g^{X-X} due to the adaptation of our InN valence band structures with the very recent results and theoretical calculations performed by King *et al.* [24], as we have already explained.

On the other hand, the effective electron mass is a fundamental quantity of semiconductors, whose knowledge is necessary for the interpretation of several experiments and theoretical models. Its value at the bottom of the conduction band (or at the top of the valence band) can be obtained from the band structure of the material under investigation using the parabolic approximation

$$\frac{1}{m^*} = \frac{4\pi^2}{h^2} \frac{\partial^2 E(k)}{\partial k^2} \quad (8)$$

We have calculated through the parabolic approximation the electronic effective mass at Γ point, but also the light hole (lh) and heavy hole (hh) effective masses along the $[1, 0, 0]$, $[1, 1, 1]$ and $[1, 1, 0]$ directions for zinc blende GaN, AlN and InN. Our obtained results are given in Table 4 in comparison with other theoretical and experimental values available in the literature. Concerning the electronic effective masses, our results agree with most references cited in Table 4. As for the hole effective masses, we remark a discrepancy between the values given by the different cited references, which prevents to assert definitely the validity of our results. Nevertheless, although we use the parabolic approximation method which is simple compared to more sophisticated methods, some of our values actually coincide with the results from other references.

3 Band structure of wurtzite nitrides

3.1 Wurtzite structure

The base vectors of the hexagonal lattice are shown in the left panel of Fig. 7: $\mathbf{a}_1 = (a, 0, 0)$, $\mathbf{a}_2 = (\frac{a}{2})(1, \sqrt{3}, 0)$ and $\mathbf{a}_3 = (0, 0, c)$ [25]. The compact hexagonal structure is made from the hexagonal lattice by placing at each site of the lattice two atoms separated by a vector $\mathbf{t} = (\frac{1}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3)$ (see middle panel of figure 7). Finally, the wurtzite structure is made from the compact hexagonal lattice by placing at each site two atoms separated by a vector $u\mathbf{a}_3$, where $u \approx 0.375$ is a parameter relative to the wurtzite structure (right panel of figure 7). Therefore, as a result, the elementary pattern of the wurtzite structure is made of 4 atoms.

The reciprocal lattice of the hexagonal lattice is also hexagonal. The base vectors of this reciprocal lattice are given by: $\mathbf{b}_1 = (\frac{2\pi}{a\sqrt{3}})(\sqrt{3}, 1, 0)$, $\mathbf{b}_2 = (\frac{4\pi}{a\sqrt{3}})(0, 1, 0)$ and $\mathbf{b}_3 = (\frac{2\pi}{c})(0, 0, 1)$. Thus, the first Brillouin zone of the reciprocal lattice of the hexagonal structure is also hexagonal. Given the high symmetry of the Brillouin

Figure 7. Hexagonal lattice (left), compact hexagonal structure (middle) and wurtzite structure (right).

zone, the band structure calculations can be considerably reduced using the symmetry operations of the crystal. In particular, it can easily be proved that a reduced region representing $1/24^{th}$ of the Brillouin zone such as reported in the right panel of Fig. 2 is sufficient to determine the energetic structure of the wurtzite crystals. This reduced region is delimited by the following points: $\Gamma = (0, 0, 0)$ (origin), $H = (\frac{2\pi}{3a}, \frac{2\pi}{a}, \frac{2\pi}{c})$ (extremity of an edge joining two rectangular sides), $A = (0, 0, \frac{\pi}{c})$ (center of an hexagonal side), $K = (\frac{2\pi}{3a}, \frac{2\pi}{a}, 0)$ (middle of an edge joining two rectangular sides), $L = (0, \frac{2\pi}{a}, \frac{2\pi}{c})$ (middle of an edge joining an hexagonal and a rectangular side), and $M = (0, \frac{2\pi}{a}, 0)$ (center of a rectangular side).

3.2 Semi-empirical pseudopotential calculation for wurtzite nitrides

The elementary pattern of the wurtzite structure is made of 4 atoms (see right panel of figure 3). By considering the origin at the center of the parallelogram formed by these atoms, their positions according to the base vectors ($\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$) are given by: $\mathbf{r}_1 = (-\frac{1}{6} - \frac{1}{6}, -\frac{1}{4} - \frac{u}{2})$, $\mathbf{r}_2 = (\frac{1}{6}, \frac{1}{6}, \frac{1}{4} - \frac{u}{2})$, $\mathbf{r}_3 = (-\frac{1}{6}, -\frac{1}{6}, -\frac{1}{4} + \frac{u}{2})$ and $\mathbf{r}_4 = (\frac{1}{6}, \frac{1}{6}, \frac{1}{4} + \frac{u}{2})$. Let $\mathbf{d}_1 = \mathbf{r}_1 - \mathbf{r}_4$ and $\mathbf{d}_2 = \mathbf{r}_2 - \mathbf{r}_3$. According to the unit vectors ($\mathbf{i}, \mathbf{j}, \mathbf{k}$), the expressions of $\mathbf{d}_1$ and $\mathbf{d}_2$ become: $\mathbf{d}_1 = (\frac{1}{4}, \frac{\sqrt{3}}{12}, \frac{1+2u}{\sqrt{6}})a$, and $\mathbf{d}_2 = (\frac{1}{4}, \frac{\sqrt{3}}{12}, \frac{1-2u}{\sqrt{6}})a$.

Because the atoms at positions $\mathbf{r}_1$ and $\mathbf{r}_2$ are identical (same atomic pseudopotential V_1), and the atoms at positions $\mathbf{r}_3$ and $\mathbf{r}_4$ are also identical (same atomic pseudopotential V_2), the expression of the pseudopotential is given by: $V_{\Delta\mathbf{g}} = V_1(\exp i\Delta\mathbf{g} \cdot \mathbf{r}_1 + \exp i\Delta\mathbf{g} \cdot \mathbf{r}_2) + V_2(\exp i\Delta\mathbf{g} \cdot \mathbf{r}_3 + \exp i\Delta\mathbf{g} \cdot \mathbf{r}_4)$. The calculation leads to the final expression:

$$V(|\Delta\mathbf{g}|) = V^s(|\Delta\mathbf{g}|)S^s(|\Delta\mathbf{g}|) + iV^a(|\Delta\mathbf{g}|)S^a(|\Delta\mathbf{g}|) \quad (9)$$

where S^s and S^a are the symmetrical and antisymmetrical structure factors with:

$$S^s = \cos[2\pi(\frac{\Delta l}{6} + \frac{\Delta m}{6} + \frac{\Delta n}{4})] \cos(\pi u \Delta n) \quad (10)$$

and

$$S^a = \cos[2\pi(\frac{\Delta l}{6} + \frac{\Delta m}{6} + \frac{\Delta n}{4})] \sin(\pi u \Delta n) \quad (11)$$

and where V^s and V^a are the symmetrical and antisymmetrical pseudopotential form factors.

A vector of the reciprocal lattice can be expressed as: $\mathbf{g} = \frac{2\pi}{a}(l\mathbf{i} + \frac{2m-l}{\sqrt{3}}\mathbf{j} + \sqrt{\frac{3}{8}}\mathbf{k})$. Its norm is therefore given

Table 5. Pseudopotential form factors (in Ry) of wurtzite GaN, AlN and InN used in the calculation. The values of $|\mathbf{G}|^2$ are given in units of $(2\pi/a)^2$.

$ \mathbf{G} ^2$		$1\frac{1}{3}$	$1\frac{1}{2}$	$1\frac{17}{24}$	$2\frac{5}{6}$	4	$4\frac{17}{24}$	$5\frac{1}{3}$	$5\frac{1}{2}$	$5\frac{17}{24}$	6	$6\frac{5}{6}$	$7\frac{1}{3}$
GaN	$\mathbf{V}_G^s$	-0.348	-0.371	-0.280	-0.053	0.059	0.083	0.056	0.066	0.067	0	0.021	0
	$\mathbf{V}_G^a$	0	0.276	0.225	0.110	0	0.051	0	0.036	0.033	0.0065	0.005	0.002
AlN	$\mathbf{V}_G^s$	-0.363	-0.321	-0.130	-0.153	0.034	0.187	0.076	0.066	0.058	0	0.121	0
	$\mathbf{V}_G^a$	0	0.476	0.125	0.310	0	-0.051	0	0.034	0.033	0.012	0.005	-0.013
InN	$\mathbf{V}_G^s$	-0.288	-0.255	-0.217	-0.010	0.044	0.056	0.025	0.015	0.036	0	-0.006	0
	$\mathbf{V}_G^a$	0	0.251	0.274	0.109	0	-0.032	0	0.029	0.0205	0.0125	0.016	-0.066

Table 6. Eigenenergies (in eV and with respect to Γ_6^v) of wurtzite GaN, AlN and InN. Our calculations are evidenced by the asterisk. All other values have been taken from the literature.

	GaN	AlN	InN
$\mathbf{K}_1^v$	-5.43 [*] , ^[16] , -5.37 ^[44] , -5.47 ^[56] , -5.6(-6.1) ^[28]	-4.66 [*] , -4.9(-5.6) ^[28]	-5.00 [*] , -5.1 ^[24]
$\mathbf{K}_3^v$	-5.26 [*] , -5.25 ^[16] , -5.29 ^[44] , -5.24 ^[56] , -5.5(-6.1) ^[28]	-4.52 [*] , -3.9(-4.5) ^[28]	-4.93 [*] , -4.9 ^[24]
$\mathbf{K}_2^v$	-3.37 [*] , -3.44 ^[16] , -2.80 ^[44] , -2.85 ^[56] , -3.0(-3.2) ^[28]	-2.90 [*] , -2.5(-3.0) ^[28]	-2.82 [*] , -2.7 ^[24]
$\mathbf{K}_3^v$	-2.92 [*] , -2.77 ^[16] , -3.02 ^[44] , -2.96 ^[56] , -3.2(-3.5) ^[28]	-2.51 [*] , -2.5(-2.9) ^[28]	-2.57 [*] , -2.6 ^[24]
$\mathbf{K}_2^c$	6.35 [*] , ^[57] , 6.70 ^[16] , 4.93 ^[44] , 7.59 ^[58] , 4.9(6.6) ^[28] , 6.6004 ^[17] , 5.74(6.97) ^[56] , 6.97 ^[59]	7.94 [*] , 6.43 ^[58] , 6.29 ^[57] , 7.3 ^[59] , 5.18 [*] , 7.0908 ^[17] , 4.8(6.7) ^[28]	
$\mathbf{M}_1^v$	-6.55 [*] , -6.52 ^[16] , -6.56 ^[44] , -6.49 ^[56] , -6.8(-7.4) ^[28]	-5.63 [*] , -5.6(-6.3) ^[28]	-5.46 [*] , -6.0 ^[24]
$\mathbf{M}_3^v$	-5.61 [*] , -5.59 ^[16] , -5.35 ^[44] , -5.32 ^[56] , -5.6(-6.1) ^[28]	-4.82 [*] , -4.3(-4.9) ^[28]	-4.65 [*] , -5.0 ^[24]
$\mathbf{M}_1^v$	-4.09 [*] , -3.88 ^[16] , -4.25 ^[44] , -4.18 ^[56] , -4.4(-4.9) ^[28]	-3.52 [*] , -3.4(-4.0) ^[28]	-4.29 [*] , -4.0 ^[24]
$\mathbf{M}_2^v$	-2.79 [*] , ^[16] , -2.57 ^[44] , -2.75 ^[56] , -2.8(-3.1) ^[28]	-2.40 [*] , -2.2(-2.6) ^[28]	-2.68 [*] , -2.6 ^[24]
$\mathbf{M}_3^v$	-2.15 [*] , -2.01 ^[16] , -2.29 ^[44] , -2.14 ^[56] , -2.4(-2.6) ^[28]	-1.85 [*] , -1.8(-2.1) ^[28]	-2.41 [*] , -2.0 ^[24]
$\mathbf{M}_4^v$	-1.09 [*] , -1.12 ^[16] , -0.88 ^[44] , -0.93 ^[56] , -1.0(-1.1) ^[28]	-0.94 [*] , -0.7(-0.9) ^[28]	-0.91 [*] , -1.0 ^[24]
$\mathbf{M}_1^c$	5.43 [*] , 5.49 ^[16] , 6.5777 ^[17] , 5.02 ^[44] , 5.94 ^[57] , 5.22(6.45) ^[56] , 5.1(6.5) ^[28] , 7.35 ^[58] , 6.45 ^[59]	7.39 [*] , 7.03 ^[58] , 6.82 ^[57] , 7.62 ^[59] , 3.52 [*] , 7.7826 ^[17] , 5.5(7.4) ^[28]	
$\mathbf{A}_{1,3}^v$	-4.18 [*] , -3.97 ^[16] , -4.06 ^[44] , -3.86 ^[60] , -4.1(-4.6) ^[28]	-3.64 [*] , -3.4(-3.9) ^[28]	-4.30 [*] , -3.8 ^[24]
$\mathbf{A}_{5,6}^v$	-0.55 [*] , ^[16] , -0.49 ^[44] , -0.52 ^[60] , -0.5(-0.6) ^[28]	-0.49 [*] , -0.6(-0.7) ^[28]	-0.56 [*] , -0.5 ^[24]
$\mathbf{A}_{1,3}^c$	5.37 [*] , 5.31 ^[16] , 5.00 ^[44] , 5.58 ^[60] , 5.31 ^[57] , 4.6(6.1) ^[28] , 6.46 ^[58] , 5.8915 ^[17]	7.35 [*] , 7.67 ^[58] , 7.78 ^[57] , 3.39 [*] , 8.1610 ^[17] , 8.13 ^[61] , 9.06 ^[62, 63] , 6.1(8.3) ^[28]	
$\mathbf{H}_3^v$	-5.98 [*] , ^[60] , -5.93 ^[16] , -6.22 ^[44] , -6.4(-7.1) ^[28]	-5.14 [*] , -5.0(-5.6) ^[28]	-5.34 [*] , -5.6 ^[24]
$\mathbf{H}_{1,2}^v$	-4.55 [*] , -4.54 ^[16] , -4.35 ^[44] , -3.85 ^[60] , -4.6(-4.9) ^[28]	-3.92 [*] , -4.0(-4.6) ^[28]	-3.67 [*] , -3.8 ^[24]
$\mathbf{H}_3^v$	-1.43 [*] , -1.40 ^[16] , -1.35 ^[44] , -1.36 ^[60] , -1.5(-1.6) ^[28]	-1.22 [*] , -0.8(-1.0) ^[28]	-1.78 [*] , -1.5 ^[24]
$\mathbf{H}_3^c$	7.62 [*] , 7.89 ^[16] , 6.62 ^[44] , 7.47 ^[57] , 8.74 ^[58] , 6.6(8.3) ^[28] , 8.5073 ^[17]	8.71 [*] , 9.19 ^[58] , 8.56 ^[57] , 4.12 [*] , 9.6651 ^[17] , 10.38 ^[61] , 9.96 ^[62, 63] , 7.2(9.5) ^[28]	
$\mathbf{L}_{1,3}^v$	-6.60 [*] , -6.57 ^[16] , -6.75 ^[44] , -6.34 ^[60] , -7.0(-7.6) ^[28]	-5.70 [*] , -5.7(-6.5) ^[28]	-5.72 [*] , -6.0 ^[24]
$\mathbf{L}_{2,4}^v$	-2.05 [*] , -2.06 ^[16] , -1.84 ^[44] , -1.76 ^[60] , -2.0(-2.2) ^[28]	-1.79 [*] , -1.5(-1.8) ^[28]	-2.07 [*] , -1.9 ^[24]
$\mathbf{L}_{1,3}^v$	-2.00 [*] , -1.95 ^[16] , -1.81 ^[44] , -1.71 ^[60] , -2.0(-2.2) ^[28]	-1.72 [*] , -1.4(-1.7) ^[28]	-1.73 [*] , -1.8 ^[24]
$\mathbf{L}_{1,3}^c$	5.52 [*] , 5.66 ^[16] , 4.54 ^[44] , 5.53 ^[60] , 5.49 ^[57] , 4.4(6.0) ^[28] , 6.71 ^[58] , 5.9506 ^[17]	7.44 [*] , 7.1549 ^[17] , 6.64 ^[58] , 3.04 [*] , 7.82 ^[63, 62] , 6.6 ^[57] , 5.0(6.9) ^[28]	

by:

$$|\mathbf{g}|^2 = \left(\frac{2\pi}{a}\right)^2 \left[\frac{4}{3}(l^2 + m^2 - ml) + \frac{3}{8}n^2\right] \quad (12)$$

Therefore, the reciprocal lattice vectors in increasing order of the modulus are in units of $(2\pi/a)$:

- $\mathbf{g}_0 \equiv (0, 0, 0)$
- $\mathbf{g}_{\frac{3}{8}} \equiv (0, 0, \pm 1)$
- $\mathbf{g}_{1+\frac{1}{3}} \equiv (-1, -1, 0), (-1, 0, 0), (0, -1, 0), (0, 1, 0), (1, 0, 0), (1, 1, 0)$
- $\mathbf{g}_{1+\frac{1}{2}} \equiv (0, 0, \pm 2)$
- $\mathbf{g}_{1+\frac{17}{24}} \equiv (\pm 1, 0, \pm 1), (0, \pm 1, \pm 1), (-1, -1, -1), (1, 1, 1), (-1, -1, 1), (1, 1, -1)$
- $\mathbf{g}_{2+\frac{5}{6}} \equiv (0, \pm 1, \pm 2), (\pm 1, 0, \pm 2), (-1, -1, -2), (1, 1, 2), (-1, -1, 2), (1, 1, -2)$
- $\mathbf{g}_{3+\frac{3}{8}} \equiv (0, 0, \pm 3)$
- $\mathbf{g}_4 \equiv (1, 2, 0), (-1, -2, 0), (2, 1, 0), (-2, -1, 0), (-1, 1, 0), (1, -1, 0)$
- $\mathbf{g}_{4+\frac{3}{8}} \equiv (1, -1, \pm 1), (-1, 1, \pm 1), (1, 2, \pm 1), (-1, -2, \pm 1), (2, 1, \pm 1), (-2, -1, \pm 1)$
- $\mathbf{g}_{4+\frac{17}{24}} \equiv (0, \pm 1, \pm 3), (\pm 1, 0, \pm 3), (-1, -1, -3), (1, 1, 3), (-1, -1, 3), (1, 1, -3)$
- $\mathbf{g}_{5+\frac{1}{3}} \equiv (\pm 2, 0, 0), (0, \pm 2, 0), (2, 2, 0), (2, 2, 0)$
- $\mathbf{g}_{5+\frac{1}{2}} \equiv (1, -1, \pm 2), (-1, 1, \pm 2), (2, 1, \pm 2), (1, 2, \pm 2), (-2, -1, \pm 2), (-1, -2, \pm 2)$
- $\mathbf{g}_{5+\frac{17}{24}} \equiv (\pm 2, 0, \pm 1), (0, \pm 2, \pm 1), (2, 2, 1), (-2, -2, 1), (2, 2, -1), (-2, -2, -1)$
- $\mathbf{g}_6 \equiv (0, 0, \pm 4)$
- $\mathbf{g}_{6+\frac{5}{6}} \equiv (\pm 0, \pm 2, \pm 2), (\pm 2, \pm 0, \pm 2), (2, 2, 2), (-2, -2, 2), (2, 2, -2), (-2, -2, -2)$
- $\mathbf{g}_{7+\frac{1}{3}} \equiv (\pm 1, \pm 0, \pm 4), (\pm 0, \pm 1, \pm 4), (-1, -1, -3), (1, 1, 3), (-1, -1, 3), (1, 1, -3)$
- $\mathbf{g}_{7+\frac{3}{8}} \equiv (-1, 1, \pm 3), (1, -1, \pm 3), (2, 1, \pm 3), (1, 2, \pm 3), (-2, -1, \pm 3), (-1, -2, \pm 3) \dots$

We neglect the pseudopotential form factors corresponding to $\mathbf{g}_0$ and to $\mathbf{g}^2 > (7 + \frac{1}{3})(\frac{2\pi}{a})^2$. Besides, we can easily verify that the term $\cos[2\pi(\frac{\Delta l}{6} + \frac{\Delta m}{6} + \frac{\Delta n}{4})]$ corresponding to the groups of vectors $\mathbf{g}_{\frac{3}{8}}, \mathbf{g}_{3+\frac{3}{8}}$ and $\mathbf{g}_{4+\frac{3}{8}}$ is always null. This is the reason why the symmetrical ($S^s(|\Delta \mathbf{g}|)$) and antisymmetrical ($S^a(|\Delta \mathbf{g}|)$) structure factors for these groups of vectors are always null.

Thus, only 12 groups of vectors remain for the calculation ($\mathbf{g}_{1+\frac{1}{3}}, \mathbf{g}_{1+\frac{1}{2}}, \mathbf{g}_{1+\frac{17}{24}}, \mathbf{g}_{2+\frac{5}{6}}, \mathbf{g}_4, \mathbf{g}_{4+\frac{17}{24}}, \mathbf{g}_{5+\frac{1}{3}}, \mathbf{g}_{5+\frac{1}{2}}, \mathbf{g}_{5+\frac{17}{24}}, \mathbf{g}_6, \mathbf{g}_{6+\frac{5}{6}}, \mathbf{g}_{7+\frac{1}{3}}$), which means 24 pseudopotential form factors: 12 symmetrical and 12 antisymmetrical. In Table 5 are given the pseudopotential form factors for wurtzite GaN and InN that we recommend and that we used in our calculations. The values of the lattice constants a and c that we used in the calculations are: $a = 0.3189$ and $c = 0.5185$ nm for GaN

[16, 64], $a = 0.3110$ and $c = 0.4980$ nm [65, 15] for AlN and $a = 0.354$ and $c = 0.570$ nm [16, 64] for InN.

Therefore, the diagonal elements of the matrix H are given by:

$$H_{i,i} = \left(\frac{\hbar^2}{2m}\right)|\mathbf{k} + \mathbf{g}_i|^2 \quad (13)$$

and the non-diagonal elements are given by:

$$H_{i,j} = V_s \cos\left(\frac{\Delta l}{6} + \frac{\Delta m}{6} + \frac{\Delta n}{4}\right) \cos(\pi \Delta n u) + iV_a \cos\left(\frac{\Delta l}{6} + \frac{\Delta m}{6} + \frac{\Delta n}{4}\right) \sin(\pi u \Delta n) \quad (14)$$

As in the zinc blende structure, we have to choose a maximum value to limit the norm, given by (12), of the reciprocal vectors that are taken into consideration in the calculation. In our case, we have verified that the condition $|\mathbf{g}|^2 < 8(\frac{2\pi}{a})^2$ (corresponding to 135 vectors) provides sufficiently accurate results. Using (13) and (14), we can calculate all the elements of the Hamiltonian matrix whose diagonalization gives the eigenvalues of the electronic states corresponding to the vector $\mathbf{k}$ of the Brillouin zone.

3.3 Results

In figures 8, 9 and 10, the energetic band structures obtained by our pseudopotential calculations are represented for wurtzite GaN, AlN and InN respectively, along the high-symmetry points Γ , K , M , A , H and L of the Brillouin zone.

Figure 8. Band structure of wurtzite GaN obtained by our pseudopotential calculations.

From a qualitative point of view, the overall shape of the valence and conduction bands of wurtzite GaN and/or AlN is similar to that obtained by the calculations performed by Yeo *et al.* [16], Fritsch *et al.* [18], Deibuk *et al.* [68], Al-Douri *et al.* [37], Goano *et al.* [17], Foley *et al.* [19], Christensen *et al.* [57], Rubio *et al.* [28], Pugh *et al.* [15], Wang *et al.* [38], Rezaei *et al.* [66]. The same occurs for wurtzite InN whose overall shape of the valence and/or conduction bands is similar to the reexamined band structures of Fritsch *et al.* [23] and King *et al.* [24].

The obtained energy eigenvalues are given in Table 6 for the high-symmetry points K , M , A , H and L . All

Table 7. Energy spacings, with respect to Γ_6^v , of wurtzite GaN, AlN and InN for the high-symmetry points Γ , L , M , H and K . Our calculations are evidenced by the asterisk, while all other values have been taken from the literature. All values are in eV.

	GaN	AlN	InN
$\Gamma_1^c - \Gamma_6^v$	3.45 [*] , 3.5036 ^[66] , 3.503 ^[67, 68] , 3.44 ^[57, 58] , 3.6 ^[69] , 3.47(3.47) ^[18] , 3.51 ^[15] , 3.5211 ^[17] , 3.36 ^[38] , 3.35 ^[46] , 3.65 ^[59] , 2.76 ^[44] , 2.89 ^[48] , 2.71 ^[70] , 3.0 ^[43] , 3.0 ^[71, 72] , 3.50 ^[73, 74, 60, 16]	6.20 [*] , 6.28 ^[75, 63, 59] , 6.2196 ^[66] , 6.24 ^[15] , 6.2 ^[61, 62, 63] , 5.8369 ^[17] , 6.11(6.11) ^{citefritsch} , 6.2 — 6.3 ^[74] , 4.84 ^[58] , 6.05 ^[57] , 5.84 ^[17] , 6.21 ^[68] , 6.20 ^[76] , 6.29 ^[77] , 4.64 ^[70]	0.70 [*] , 0.824(0.790) ^[23] , 0.8 ^[20, 22] , 0.7 ^[21]
$\Gamma_6^v - \Gamma_3^v$	6.63 [*] , 6.816 ^[66] , 8.0135 ^[17] , 6.94(6.97) ^[18] , 7 ^[78] , 6.8 ^[16] , 6.78 ^[60] , 7.18 ^[44] , 7.21 ^[79] , 7.0 ^[72]	6.70 [*] , 6.2136 ^[66] , 6 ^[80] , 7.0061 ^[17] , 6.41(6.44) ^[18]	6.33 [*] , 6.024(6.154) ^[23] , 6.10 ^[81]
$\Gamma_5^v - \Gamma_6^v$	1.08 [*] , 1.00(1.00) ^[18] , 1.00 ^[72]	0.92 [*] , 1.03(1.04) ^[18]	1.03 [*] , 1.022(1.037) ^[23]
$\Gamma_6^v - \Gamma_3^c$	4.99 [*] , 4.97 ^[16] , 4.68 ^[60] , 4.76 ^[44] , 5.8735 ^[17]	7.92 [*] , 8.2907 ^[17]	2.81 [*]
$\Gamma_5^v - \Gamma_3^c$	6.07 [*] , 5.96(5.96) ^[18] , 5.28 ^[68] , 5.3 ^[69] , 5.9 ^[72]	8.84 [*] , 8.94(8.95) ^[18] , 8.63 ^[68] , 8.92 ^[76] , 8.02 ^[77]	3.84 [*] , 3.581(3.602) ^[23]
$\Gamma_5^v - \Gamma_6^c$	10.48 [*] , 10.74(10.74) ^[18] , 11.1 ^[72]	13.03 [*] , 12.97(12.99) ^[18] , 14.00 ^[77]	10.15 [*] , 9.822(9.859) ^[23]
$L_{2,4}^v - L_{1,3}^c$	7.57 [*] , 7.34 ^[38] , 7.29 ^[69] , 7.24 ^[60] , 7.57 ^[16] , 7.05 ^[70]	9.23 [*]	5.11 [*] , 5.216(5.245) ^[23] , 5.41 ^[81]
$M_4^v - M_1^c$	6.52 [*] , 6.60 ^[38] , 6.07(6.07) ^[18] , 7.0 ^[46] , 7.05 ^[60] , 6.61 ^[16] , 6.7 ^[70]	8.33 [*] , 7.87(7.88) ^[18]	4.43 [*] , 4.522(4.556) ^[23]
$M_4^v - M_3^c$	7.54 [*] , 7.47 ^[38] , 7.68(7.68) ^[18] , 7.3 ^[60] , 7.69 ^[16] , 7.25 ^[70] , 6.8 ^[68] , 7.0 — 7.1 ^[69]	8.94 [*] , 8.83(8.81) ^[18] , 9.7 ^[68]	5.12 [*] , 5.101(5.134) ^[23]
$M_2^v - M_1^c$	8.22 [*] , 8.35 ^[38] , 7.9 ^[46] , 8.5 ^[60] , 8.26 ^[16] , 7.13 ^[68] , 7.0 — 7.1 ^[69] , 7.67(7.67) ^[18]	9.79 [*] , 10.24 ^[68] , 8.21 ^[76] , 9.54(9.56) ^[18]	6.20 [*] , 6.090(6.142) ^[23] , 6.10 ^[81]
$H_3^v - H_3^c$	9.05 [*] , 8.04 ^[38] , 8.4 ^[60] , 8.07(8.06) ^[18] , 9.0 ^[16]	9.93 [*] , 10.91(10.10) ^[18] , 10.39 ^[77]	5.90 [*] , 5.892(5.883) ^[23] , 6.10 ^[81]
$K_2^v - K_2^c$	9.72 [*] , 9.12 ^[38] , 8.68(8.68) ^[18] , 9.0 ^[46] , 9.45 ^[60] , 10.1 ^[16] , 9.82 ^[56] , 8.3 ^[72]	10.84 [*] , 9.57(9.59) ^[18]	8.00 [*] , 8.028(8.141) ^[23]
$K_3^v - K_2^c$	9.27 [*] , 9.08 ^[38] , 8.55(8.54) ^[18] , 9.05 ^[60] , 9.43 ^[16] , 8.29 ^[68] , 8.3 — 8.7 ^[69] , 7.9 ^[72]	10.45 [*] , 9.43(9.43) ^[18] , 10.84 ^[68] , 7.90 ^[76]	7.75 [*] , 7.617(7.550) ^[23]

Table 8. Effective masses of wurtzite GaN, AlN and InN. Our calculations are evidenced by the asterisk, while all other values have been taken from the literature. All values are in units of the free electron mass.

	GaN	AlN	InN
$m_e^{\parallel}$	0.1712*, 0.16 ^[15] , 0.18 ^[82] , 0.20 ^[42, 48] , 0.20(0.20) ^[79] , 0.19(0.19) ^[16, 83] , 0.138(0.138) ^[18] , 0.14(0.14) ^[84] , 0.2 ^[85] , 0.1846 ^[17] , 0.189 ^[60] , 0.27 ^[70] , 0.197 ^[86]	0.3006*, 0.232(0.231) ^[18] , 0.33(0.33) ^[79] , 0.24(0.24) ^[84]	0.1076*, 0.069(0.072) ^[23] , 0.07 ^[52]
$m_e^{\perp}$	0.1253*, 0.12 ^[15] , 0.20 ^[42] , 0.2 ^[85] , 0.17(0.17) ^[16] , 0.151(0.151) ^[18] , 0.18(0.18) ^[79] , 0.15(0.15) ^[84] , 0.2283 ^[17] , 0.221 ^[60] , 0.33 ^[70] , 0.22 ^[48] , 0.198 ^[86] , 0.23(0.19) ^[83]	0.2351*, 0.242(0.242) ^[18] , 0.25(0.25) ^[79] , 0.25(0.25) ^[84]	0.0767*, 0.069(0.068) ^[23] , 0.07 ^[52]
$m_{hh}^{\parallel} = m_{lh}^{\parallel}$	1.9299*, 2.00(1.96) ^[83] , 1.89 ^[87] , 2.007(2.000) ^[18] , 1.453(1.479) ^[84] , 1.76(1.10) ^[79] , 1.76(1.96) ^[16] , 1.27 ^[15] , 2.12 ^[82]	2.3595*, 2.382(2.370) ^[18] , 3.53(3.68) ^[79] , 1.869(1.949) ^[84] , 3.53(4.41) ^[83]	1.5564*, 2.631(2.566) ^[23] , 1.563 ^[52]
$m_{ch}^{\parallel}$	0.1462*, 0.14 ^[15] , 0.16 ^[82] , 0.12 ^[87] , 0.130(0.130) ^[18] , 0.125(0.130) ^[84] , 0.16(0.15) ^[79] , 0.14(0.14) ^[16] , 0.16(0.16) ^[83]	0.1788*, 0.209(0.209) ^[18] , 0.25(0.25) ^[79] , 0.26(0.27) ^[83] , 0.212(0.229) ^[84]	0.1506*, 0.080(0.071) ^[23] , 0.122 ^[52]
$m_{hh}^{\perp}$	2.0264*, 2.00 ^[87] , 2.04(1.20) ^[83] , 2.249(2.255) ^[18] , 1.595(1.592) ^[84] , 1.61(1.65) ^[79] , 1.69(1.87) ^[16] , 2.27 ^[82] , 1.02 ^[15]	2.4775*, 3.040(3.058) ^[18] , 10.42(6.33) ^[79] , 2.421(2.584) ^[84] , 11.14(2.18) ^[83]	2.1638*, 2.889(2.967) ^[23] , 1.250 ^[52]
$m_{lh}^{\perp}$	0.1425*, 0.15 ^[87] , 0.14(0.15) ^[79] , 0.261(0.191) ^[18] , 0.236(0.299) ^[84] , 0.14(0.14) ^[16] , 0.18(0.16) ^[83] , 0.11 ^[15] , 0.20 ^[82]	0.1743*, 0.287(0.285) ^[18] , 0.24(0.25) ^[79] , 0.252(0.350) ^[84] , 0.33(0.29) ^[83]	0.1252*, 0.107(0.071) ^[23] , 0.091 ^[52]
$m_{ch}^{\perp}$	2.2854*, 1.36 ^[15] , 1.25 ^[82] , 0.59 ^[87] , 0.317(0.567) ^[18] , 1.04(1.10) ^[79] , 0.289(0.252) ^[84] , 1.76(1.96) ^[16] , 1.49(1.96) ^[83]	2.7942*, 1.157(1.204) ^[18] , 3.81(3.68) ^[51] , 1.484(0.709) ^[84] , 4.05(4.41) ^[83]	0.7906*, 1.191(1.244) ^[23] , 1.471 ^[52]

Figure 9. Band structure of wurtzite AlN obtained by our pseudopotential calculations.

eigenvalues are given with respect to the top of the valence band Γ_6^v . First we notice that, as for zinc blende InN, all results and calculations before 2002 that do not take into consideration the new corrections brought into the band structure of wurtzite InN have not been included in our comparison. In addition, the values corresponding to ref. [24] are approximate values that we have estimated from the band structure of wurtzite InN obtained by King *et al.* [24], since no accurate values are available in the article, but only the obtained band structure. Note that, in Table 6 and for the reference [28] (Rubio *et al.*), there are two proposed values for each energy eigenvalue, both calculated using the LDA method, but the value in parenthesis is the result of an additional correction that takes into consideration the electrons screening effect via the Green function (GW approach) [28]. Similarly, there are two values for the reference [56] (Lambrecht *et al.*): the second value in parenthesis corresponds to a correction due to the LMTO-LDA approach (linear muffin-tin orbital). An overview of the table shows a satisfactory general agreement with the results of most cited references [17, 24, 28, 44, 56, 57, 58, 59, 60].

Figure 10. Band structure of wurtzite InN obtained by our pseudopotential calculations.

To ensure the accuracy of our semi-empirical results in comparison with experimental and other *ab-initio* and semi-empirical results, the values of energy spacings at high symmetry points Γ , L , M , H and K are given in

Table 7. In particular, the energy spacings $\Gamma_1^c - \Gamma_6^v$ and $\Gamma_6^v - \Gamma_3^v$ represent the bandgap E_g and the valence band width respectively. Note that in Table 7, the calculations made by Fritsch *et al.* [18, 23] propose two values for each energy spacing: the first corresponds to a calculation from an isotropic model of the screening effect, whereas the second value in parenthesis corresponds to an anisotropic correction of the screening effect. The validity of our semi-empirical calculations and our chosen pseudopotential form factors is well verified by the agreement of our obtained GaN and/or AlN energy spacings with other calculations, like the calculations made by Yeo *et al.* [16], Fritsch *et al.* [18], Wang *et al.* [38] and others. Furthermore, our chosen pseudopotential form factors are well adapted to the latest experimental and theoretical results that take into consideration the band gap corrections of wurtzite InN [20, 21, 22, 23].

A parabolic line fit is also used to determine the effective masses of the electrons for wurtzite GaN, AlN and InN. The lowermost conduction band shows slight anisotropy for $\mathbf{k}$ directions. For GaN, $m_e^{\parallel} = 0.1712m_0$ in the k_z direction, and $m_e^{\perp} = 0.1253m_0$ in the k_xk_y plane. For AlN, $m_e^{\parallel} = 0.3006m_0$ in the k_z direction, and $m_e^{\perp} = 0.2351m_0$ in the k_xk_y plane. For InN, $m_e^{\parallel} = 0.1076m_0$ in the k_z direction, and $m_e^{\perp} = 0.0767m_0$ in the k_xk_y plane. Our results along with other available data in the literature are shown in Table 8. Note first that in Table 8, regarding the results of Fritsch *et al.* [18, 23], there are two proposed values for each of the calculated effective masses, the value in parenthesis corresponds to an additional anisotropic correction. Dudgale *et al.* [84] also propose two values: the first is calculated directly by the $\mathbf{k} \cdot \mathbf{p}$ method, the second by the Monte Carlo method. Similarly, there are two values proposed by Suzuki *et al.* [79] for each of the effective masses, the second in brackets resulting in a further correction by a 3D interpolation procedure within the cubic approximation. As for Yeo *et al.* [16] values, one comes from the parabolic approximation, the other is due to the $\mathbf{k} \cdot \mathbf{p}$ method. Finally, the second value given by Kim *et al.* [83] is obtained through a quasicubic model calculation. The discrepancy between the values given by the cited references does not preclude the fact that our values are consistent with several values proposed by other calculations, especially those of Ren *et al.* [87], but also those of Fritsch *et al.* [18, 23] and Yeo *et al.* [16], despite the use of different approximations and calculation methods.

4 Comparative analysis

In Table 9 the main characteristics and parameters that we can deduce from the energetic band structures of GaN, AlN and InN are grouped for both zinc blende and wurtzite phases. In particular, we have reported the bandgap value but also other important parameters such as the effective masses, the nonparabolicity coefficient of the Γ valley and the valence band width. The results show that zinc blende GaN and InN are direct-gap semiconductors with the minimum of the conduction band at Γ point, whereas zinc blende AlN has an indirect gap with the minimum of conduction band at

Table 9. Comparison of the main parameters of GaN, AlN and InN in both zinc blende and wurtzite phases. All energetic values are in eV. All effective masses are in units of the free electron mass m_0 . The nonparabolicity coefficient is given in eV^{-1} .

	GaN		AlN		InN	
	ZB	WZ	ZB	WZ	ZB	WZ
Direct/indirect gap	direct	direct	indirect	direct	direct	direct
Bandgap value	3.23	3.45	4.91	6.21	0.51	0.70
Valence band width	6.15	6.63	5.86	6.70	6.51	6.33
Effective masses	m_e	0.1393	0.271		0.1140	
	$m_e^{\parallel}$	0.1712		0.3006		0.1076
	$m_e^{\perp}$	0.1253		0.2351		0.0767
Nonparabolicity coefficient	0.229	0.199	0.090	0.079	1.539	1.138

X point. The calculated values of the bandgap $E_g^{\Gamma-\Gamma}$ of GaN and InN are 3.23 and 0.51 eV respectively, and the bandgap $E_g^{\Gamma-X}$ of AlN is equal to 4.91 eV. These values are in good agreement with other experimental and theoretical results, as we have already shown in Table 3. As for wurtzite GaN, AlN and InN, they are direct-gap semiconductors with the minimum of conduction band at Γ point. The values of our calculated bandgaps for wurtzite GaN, AlN and InN are 3.45, 6.20 and 0.70 eV respectively, thus covering a wide energy range of the electromagnetic spectrum and as a consequence more potential applications. On the other hand, all studied nitrides have similar values of the valence band width (≈ 6 eV) and AlN in both its zinc blende and wurtzite phases has a larger effective mass than GaN and InN. Finally, we have also calculated the nonparabolicity coefficient α in the Γ valley of the conduction band, a very important parameter for instance in electronic devices transport simulations. It can be easily calculated using the approximation $\alpha = (1/E_g)(1 - m^*/m_0)^2$, where E_g is the bandgap value and m^* the electron effective mass in the Γ valley.

5 Conclusion

We have presented reexamined band structures for zinc blende and wurtzite InN in agreement with the latest corrections brought into its bandgap values, as well as a comparative study of the electronic band structures of zinc blende and wurtzite GaN, AlN and InN using the empirical pseudopotential approach. The obtained band structures are validated by a comparison with most of the experimental data and *ab-initio* calculations reported in the literature. GaN and InN in both zinc blende and wurtzite structures, as well as wurtzite AlN have direct bandgaps, but zinc blende AlN has an indirect gap at X point. All calculated bandgaps values are found to be in agreement with other experimental and theoretical results. In particular, zinc blende and wurtzite InN bandgap values are consistent with the latest measurements that clearly demonstrated that the bandgap value of InN is lower than 1 eV, much lower than the bandgap values of (zinc blende/wurtzite) GaN (3.23/3.45 eV) and (zinc blende/wurtzite) AlN (4.91/6.20 eV). The effective mass parameters are also derived using a parabolic fit which has proven to be a reliable approximation in most cases.

For practical purposes, all the optimized symmetrical and antisymmetrical pseudopotential form factors have

been tabulated to fill the lack in the literature regarding the empirical pseudopotential parameters of zinc blende and wurtzite III-nitrides. Furthermore, we have tabulated the eigenenergies at high-symmetry points, valley separation energies and bandgaps, electron and hole effective masses, and nonparabolicity coefficients, all of which are crucial parameters for microscopic numerical simulations of electronic and optoelectronic devices.

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