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The late 1990s mark the entrance of group-III nitride compounds and their alloys to the world of optical and electronic devices. The use of pseudobinary InGaN, AlGaN, and InAlN alloys enabled the fabrication of light-emitting diodes and laser diodes operating in the green-blue-UV spectral region and of high-frequency, high-power, and high-temperature electronic devices.1 Alloys among the group-III nitrides allow to engineer the band gap (BG) from 0.70 eV in InN to 6.28 eV in AlN with an intermediate value of 3.44 eV for GaN.2

Due to their technological importance, an accurate prediction of optical properties of group-III nitride alloys is highly desirable. Theoretical studies often utilize density functional theory (DFT) within the local density approximation (LDA), or the generalized gradient approximation (GGA).3 However, while LDA and GGA accurately predict many ground state properties, the Kohn–Sham BG’s are significantly underestimated in comparison to the experimental ones. In the extreme case of InN, the predicted BG is even negative, leading to a metal instead of a semiconductor.3 These discrepancies are caused by the lack of the discontinuity of the exchange-correlation potential. Several methods to overcome these limitations have been proposed. One of them is the GW approximation, which considers the energies of quasiparticles and calculates the electron self-energy in terms of perturbation theory.4 This procedure achieves good accuracy, but it goes beyond the DFT, and is computationally demanding, complicating its application to complex systems, like the alloys studied here. Other procedures were also proposed, among them we may cite the hybrid functionals which allows accurate calculations of the BG and were also applied to nitride systems. One example is a recent study conducted by Moses and Van de Walle considering the hybrid exchange-correlation functional of Heyd, Scuseria and Ernzerhof (HSE), and special quasi-random structures, to obtain the BG of InGaN alloys.5

Another point to be considered when dealing with alloys is the statistics: for a rigorous calculation, it is imperative to take into account different configurations within a statistical scheme.6 Therefore, to keep the computational time reasonably bounded, a reliable method for obtaining excited states at low computational costs is highly desirable. There is no theoretical work reported so far which contemplates, on an equal footing, both, a reasonably sized model supercell and the statistics of the alloy, and a method that corrects the energy gap. All of them use only one or just few alloy configurations. The method we employ here surpasses this difficulty.

Recently, Ferreira et al.7 proposed a method called LDA-1/2 which approximately includes the self-energy of excitations in semiconductors, providing BG energies, effective masses, and band structures in very good agreement with experiment. The great advantages of the method are: (i) the low computational cost, comparable to a traditional LDA calculation; (ii) the simple implementation, making the method easily applicable within several ab initio approaches, as pseudopotential calculations,8 projector augmented wave (PAW),9 linearized augmented plane wave (LAPW),10 and (iii) it has no empirically adjusted parameters. These features make LDA-1/2 a promising method for studies of large and complex semiconducting systems.12

In this work, electronic properties of wurtzite InGaN, AlGaN, and AlInN alloys are studied by combining first-principles calculations within the LDA-1/2 approach with the generalized quasichemical approach (GQCA) to include disorder and compositional effects. The BG’s and bowing parameters (BP’s) are obtained for the whole range of the alloy composition.

The GQCA is well described elsewhere,13,14 and has already been used for nitride alloys.6,14 The macroscopic alloy $A_xB_{1-x}N$ (A and B stand for Al, Ga, or In) is divided into an ensemble of clusters independent statistically and energetically of the surrounding atomic configuration. We used sixteen-atom supercells as basic clusters to describe the fully relaxed alloys. The total energy and the BG of each cluster is calculated by adopting a pseudopotential plane-wave DFT code, as implemented in the "VIENNA AB-INITIO SIMULATION
TABLE I. LP’s as recommended in Ref. 16 and band energy gaps (eV) obtained with the LDA-1/2 compared with pure LDA and experimental results of Ref. 16

<table>
<thead>
<tr>
<th>Composition</th>
<th>a (Å)</th>
<th>c (Å)</th>
<th>E_{LDA}</th>
<th>E_{LDA-1/2}</th>
<th>E_{exp}</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlN</td>
<td>3.112</td>
<td>4.982</td>
<td>4.50</td>
<td>6.06</td>
<td>6.23</td>
</tr>
<tr>
<td>GaN</td>
<td>3.189</td>
<td>5.185</td>
<td>2.02</td>
<td>3.52</td>
<td>3.507</td>
</tr>
<tr>
<td>InN</td>
<td>3.545</td>
<td>5.703</td>
<td>-0.03</td>
<td>0.95</td>
<td>0.7–1.9</td>
</tr>
</tbody>
</table>

TABLE II. BG bowing parameter (eV) for the studied alloys: results obtained from LDA and LDA-1/2 calculations, compared with those recommended by Vurgaftman et al.16

<table>
<thead>
<tr>
<th>Composition</th>
<th>LDA</th>
<th>LDA-1/2</th>
<th>Ref. 16</th>
</tr>
</thead>
<tbody>
<tr>
<td>In_{x}Ga_{1-x}N</td>
<td>1.4</td>
<td>1.3</td>
<td>1.4</td>
</tr>
<tr>
<td>Al_{x}Ga_{1-x}N</td>
<td>0.4</td>
<td>0.8</td>
<td>0.7</td>
</tr>
<tr>
<td>Al_{x}In_{1-x}N</td>
<td>2.7</td>
<td>3.4x+1.2</td>
<td>2.5</td>
</tr>
</tbody>
</table>

The LP’s recommended by Vurgaftman and Meyer16

for binary compounds AlN, GaN, and InN, we use the values for

pj

from Vegard’s law. To demonstrate the accuracy of the LDA-

and for clusters with mixed cations, the LP’s are obtained

Experimental results, as follows: a (Ref. 17), b (Ref. 18), c (Ref. 19), d (Ref. 20), e (Ref. 21), f (Ref. 22), g (Ref. 23), h (Ref. 24), i (Ref. 25), j (Ref. 26), k (Ref. 27), and l (Ref. 28).

FIG. 1. (Color online) Comparison between the energy gap of the In_{x}Ga_{1-x}N alloy calculated through the ordinary LDA exchange-correlation potential (red line) and the LDA-1/2 method (blue line). The symbols represent experimental results, as follows: a (Ref. 17), b (Ref. 18), c (Ref. 19), d (Ref. 20), e (Ref. 21), f (Ref. 22), g (Ref. 23), h (Ref. 24), i (Ref. 25), j (Ref. 26), k (Ref. 27), and l (Ref. 28).

FIG. 2. (Color online) BG of the Al_{x}Ga_{1-x}N alloy: comparison between LDA (red line) and LDA-1/2 (blue line) calculations. Experimental results: a (Ref. 29), b (Ref. 30), c (Ref. 31), and d (Ref. 32).
FIG. 3. (Color online) Energy gap of the AlInN alloy: comparison between LDA (red line) and LDA-1/2 (blue line) calculations. Experimental results: a (Ref. 33), b (Ref. 34), c (Ref. 35), d (Ref. 36), e (Ref. 37), f (Ref. 38), g (Ref. 39), h (Ref. 40), and i (Ref. 41).

LDA-1/2 for obtaining excited states within the DFT at a low computational cost. We compared our results with LDA and experimental data. The results were surprisingly good: LDA-1/2 predictions for the BG and respective BP fit remarkably well with experimental results for all alloys studied. This study shows that LDA-1/2 is a promising parameter-free method to study the properties of excited states of large and complex semiconducting systems, but at a very small computational price.

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