

Electron localization and emission mechanism in wurtzite (Al, In, Ga)N alloys

Qihang Liu^{*,1}, Jing Lu^{**,1}, Zhengxiang Gao¹, Lin Lai¹, Rui Qin¹, Hong Li¹, Jing Zhou¹, and Guangping Li²

¹State Key Laboratory for Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P.R. China ²SICAS Centre, Lee Hall, SUNY Oneonta, Oneonta, New York 13820, USA

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* Corresponding author: e-mail ferrero1985@gmail.com, Phone: +86-010-62755701, Fax: +86-010-62755701 ** e-mail jinglu@pku.edu.cn

The electronic structures of wurtzite InGaN and AlGaN alloys are investigated using the first-principle density functional theory calculation. The results indicate that some short In–N–In atomic chains and small In–N atomic condensates composed of a few In and N atoms can be randomly formed in InGaN alloys. The electrons at the top of valence bands can be effectively localized in the vicinity of the In–N–In zigzag chains (weak localization) and the In–N atomic condensates (strong localization). These localized electrons extremely enhance the emission efficiency of InGaN alloys.

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1 Introduction At present, InGaN alloys are producing blue and green light emitting diodes (LEDs) for fullcolour displays, optical storage and solid-state lighting [1–3]. Their bandgap energies can continuously vary from 0.65 eV for InN to 3.43 eV for GaN at room temperature. Therefore, InGaN alloys are natural choice of materials for light emitters that are operated in the infrared to ultraviolet range depending on their compositions. The internal quantum efficiency of the near-band-edge emission in $In_xGa_{1-x}N$ quantum wells (QWs) increases from 0.3% for x = 0 (GaN) to approximately 80% for x = 0.15 (blue LEDs) [4]. As a result, the commercially available LEDs exclusively use InGaN alloys in the active regions, although the threading dislocation density generated in these InGaN alloys due to lattice mismatch (10^9 cm^{-2}) is typically six orders of magnitude higher than that in conventional (Al,In,Ga)(As,P) LED films [5]. The coexistence of the high quantum efficiency of the photoluminescence (PL) and the high density of the threading dislocation indicates strong carrier localization. This means that an exciton is localized in space before it can reach the impurity sites to be annihilated non-radiatively. One current focus of research is to understand the mechanism of this localization.

InGaN alloys appear versatility of the alloy decomposition patterns experimentally and they are sensitive to the



particular experimental conditions. Theoretical calculations proposed by Ganchenkova et al. [6] attributed it to the high sensitivity of the InGaN decomposition to relatively small variations of the interaction between Ga and In atoms. It has been widely accepted belief that In atoms in the InGaN QWs form In-rich clusters due to the fluctuations of In compositional in the $In_xGa_{1-x}N$ layer. Many transmission electron micrograph (TEM) observations [7, 8] and systematic studies on optical properties have validated this [9, 10]. However, it is electron beam damage that produced the Inrich clusters in InGaN in the electron microscope experiment [11], and careful low-dose electron microscopy reveals no gross In clustering, but it cannot rule out small In fluctuations. Three-dimensional atom probe analysis of InGaN QWs reported by Humphreys [12] demonstrates that InGaN in the QWs is a random alloy. Chichibu et al. [13] have recently explained their positron annihilation results in InGaN that the holes (positrons) were captured by atomic condensates of In-N or In-N-In zigzag chains. The empirical pseudopotential and first-principle calculations also predicted the localization of the hole wave functions in InGaN alloys along the randomly formed In-N-In chains [14, 15]. Some other explanations such as the QW thickness fluctuation [16], strain inhomogeneity [17, 18], quantumconfined Stark effect (QCSE) [19, 20] and so on exist as well. But the emission mechanism of InGaN alloys is still in



controversy. In this work we will mainly concentrate on the electronic structures of the wurtzite InGaN alloys with different configurations (uniform, chain and atomic condensate) to investigate the electron localization and elucidate the emission mechanism of the alloys.

2 Method of calculation All calculations are performed using the Vienna ab initio simulation package (VASP) [21], which employs density functional theory (DFT) to simulate properties of a wide range of solid materials. To model $In_xGa_{1-x}N$ wurtzite alloys, we chose a 72-atom supercell, which consists of $3 \times 3 \times 2$ primitive cells. VASP implements a quantum mechanical molecular dynamic simulation algorithm, from which we have chosen the projector augmented plane wave basis functions (PAW) [22, 23]. The generalized gradient approximation with Perdew-Burke-Ernzerhof's exchange-correlation potential [24] is adopted, and the Ga 3d and In 4d electrons are treated as valence electrons. The cut-off energy is chosen as 500 eV, and the total energy is converged to less than 0.001 eV/atom. For the wurtzite structure, we use a $5 \times 5 \times 5$ Γ -centred kpoints grids for the integration of the first Brillouin zone, because standard Monkhorst-Pack grids do not have full hexagonal symmetry. Our calculations with other k meshes have proven this choice is adequate.

3 Results and discussion For the ideal wurtzite GaN, our calculations (see Table 1) provide a valence band width (VBW) of 7.03 eV, which is in excellent agreement with the experimental value of 7.0 eV [25] and other theoretical results [26, 27]. Moreover, the ideal GaN has a direct bandgap of 1.88 eV at Γ point, which is also in good agreement with previous theoretical calculations [28–30]. Compared with the experimental values [31, 32], the theoretical bandgaps are significantly underestimated. The physical reason is that the discontinuity of the exchange-correlation potential with respect to particle number in the DFT calculations, as pointed out by Seidl et al. [33].

3.1 Electronic structure and density of states of InGaN alloys In order to elucidate the emission mechanism of InGaN alloys, we will investigate the electron localization of InGaN in detail in the following sections. For simplicity, we choose the $In_5Ga_{31}N_{36}$ alloy with an indium concentration of 13.9% (close to the commonly experimental sample $In_{0.15}Ga_{0.85}N$) as model in our calculations. Twelve In configurations are divided into three classes, and

Table 1 The bandgap and valence band width (VBW) in eV in comparison with the experimental and previous theoretical results for the ideal wurtzite GaN.

	experiments	other calculations	this work
bandgap	3.44 [30], 3.50 [31]	1.86 [27], 1.9 [28], 1.92 [29]	1.88
VBW	7.0 [24]	6.8 [25], 6.81 [26]	7.03

we mainly discuss the configuration that has the lowest total energy of each class. First, we investigate a homogeneous $In_5Ga_{31}N_{36}$ alloy (uniform model) with 5 In atoms distributing uniformly in a 72-atom supercell (Fig. 1a). A chain model, with 5 In atoms forming 2 In–N–In zigzag chains, is further considered (Fig. 1b). At last, we investigate a small In–N atomic condensate model with 5 In atoms congregating together (Fig. 1c). By comparing the total energy, we can find the most stable model among the three. Moreover, our goal is to provide answers to the key issue: How to realize the electron localization in InGaN alloys and what is its emission mechanism?

In gallium nitride, both the Ga and N atoms are tetrahedrally coordinated to four nearest neighbours. Three of the four bond lengths are 1.941 Å and one is 1.977 Å [34]. This symmetry breaking from T_d to C_{3V} is easily explained in terms of the sp³ hybridization of gallium and nitrogen atoms. The optimized structures for the GaN primitive cell and various In₅Ga₃₁N₃₆ models using VASP are listed in Table 2. We can see that our calculated results for the GaN primitive cell, including the lattice parameters and the Ga-N bond lengths, are in good agreement with the experiment [34]. The lattice structures expand when doped with some In atoms, and the volumes of $In_5Ga_{31}N_{36}$ supercells increase nearly 5%in comparison with Ga₃₆N₃₆. The lattice parameters have changed slightly among the three In₅Ga₃₁N₃₆ configurations. The condensate model has the largest volume, due to the interaction of the congregating In atoms. The last two columns list a range of lengths of the Ga-N and In-N bonds. In the InGaN alloys, the In atoms substituting for Ga atoms remain tetrahedrally coordinated. The lengths of the Ga-N and In-N bonds are 1.948-2.001 Å and 2.139-2.147 Å, respectively, for the uniform model; 1.952-1.981 Å and 2.127-2.148 Å, respectively, for the chain model and 1.949-1.981 Å and 2.106–2.145 Å, respectively, for the condensate model.

The total energies and band parameters for the three In configurations in the $In_5Ga_{31}N_{36}$ alloy are listed in Table 3. The uniform model has the lowest energy among the three models, and we set it as zero to make the difference clearly. It appears that in the zero temperature the most stable InGaN material is a homogeneous alloy with indium atoms distributed uniformly due to the total energy comparison. The chain model is a little higher in energy than the uniform model, while the condensate model is the least stable. However, it is interesting to note that the energy difference between the uniform and chain (condensate) models is small (0.53 eV). Therefore, both chain and condensate models do have definite probabilities to form, which means there exist many short In-N-In chains and small In-N atomic condensates in real InGaN alloys. Moreover, the bandgap of InGaN intrinsically depends on the way how In atoms are distributed in the alloy, due to the intensity of the interactions between indium atoms in various configurations.

The electronic band structures and partial density of states (PDOS) for the uniform model in the $In_5Ga_{31}N_{36}$ alloy are shown in Fig. 2. The $In_5Ga_{31}N_{36}$ uniform alloy has a



Figure 1 (online colour at: www.pss-b.com) A 72-atom supercell of the wurtzite $In_5Ga_{31}N_{36}$ with $3 \times 3 \times 2$ primitive cells for the uniform model (a), chain model (b) and condensate model (c). In, Ga and N atoms are shown as red, grey and blue spheres, respectively. The In–N–In zigzag chains and In–N atomic condensates are labelled by solid lines.

Table 2 Optimized structures for the GaN primitive cell and various $In_5Ga_{31}N_{36}$ models.

supercell	a (Å)	<i>c</i> (Å)	volume (Å ³⁾	$d_{\text{Ga-N}}$ (Å)	$d_{\text{In-N}}$ (Å)
GaNexpt	3.1891	5.185	45.67	1.942-1.977	_
Ga_2N_2	3.2144	5.247	46.94	1.967-1.971	-
In ₅ Ga ₃₁ N ₃₆ (uniform)	3.2656×3	5.317×2	883.46	1.948-2.001	2.139-2.147
$In_5Ga_{31}N_{36}$ (chain)	3.2651×3	5.321×2	884.41	1.952-1.981	2.127-2.148
In ₅ Ga ₃₁ N ₃₆ (condensate)	3.2656×3	5.319 × 2	884.56	1.949–1.981	2.106-2.145

direct bandgap of 1.29 eV at Γ point (see Fig. 2a). The band width of valence bands is 6.71 eV. Compared with the ideal GaN, our calculations also show the lift of degeneracy for both the conduction and valence bands in the InGaN alloy. There are no new bands appearing in the forbidden gap without any dispersion for this model, which indicates the presence of a localized state in the common sense. We later will only focus on the VBM and CBM states because the PL of semiconductor materials is related to the VBM and CBM states. Figure 2b clearly indicates that the VBM states have a prominent admixture of N 2p-, Ga 3d- and In 4d- and 5p-like

Table 3 Comparison of the total energy, bandgap and valenceband width (VBW) (eV) in wurtzite InGaN alloys with different Indistributions.

model	uniform	chain	condensate
total energy	0	0.10	0.53
bandgap	1.29	1.27	1.19
VBW	6.71	6.71	6.81

states. No electron localization is apparent from this uniform model. Hence the uniform model cannot improve the emission efficiency of InGaN alloys.

For the configuration with several In–N–In zigzag chains, the electronic structure (not plotted here), including the conduction bands, the valence bands and the forbidden bandgap (1.27 eV) is little different in comparison with that of the uniform model. A remarkable change is that the PDOS of the VBM states has a δ -function-like peak due to the contribution of the N (bonded with In) 2p-, In 4d- and 5p-like states. This is a direct manifestation that the electrons in the vicinity of the VBM are localized around the In–N–In zigzag chains. The In–N–In chain model is expected to improve the emission efficiency of InGaN alloys due to the electron localization along the In–N–In chains.

3.2 Electron localization in InGaN alloys The electronic band structures and PDOS of the $In_5Ga_{31}N_{36}$ with a small In–N atomic condensates are shown in Fig. 3. Compared with Fig. 2, several remarkable changes are revealed. The bandgap (1.19 eV) shrinks significantly, due to



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Figure 2 (online colour at: www.pss-b.com) Electronic band structures (a) and the corresponding PDOS (b) of the uniform wurtzite $In_5Ga_{31}N_{36}$. Here the PDOS of one In atom, one of the nearest N atoms, and a Ga atom far away is given.

the strong atomic interaction in the small In–N condensate. The band broadening of the highest valence band is reduced to 0.40 eV, less than the corresponding values of the uniform model (0.47 eV) and the chain model (0.48 eV), which correlates the overlapping of the electron wave function of the crystal. Moreover, in the PDOS of the condensate model (Fig. 3b), there is a strong mixing of atomic states from the In



Figure 3 (online colour at: www.pss-b.com) Same as in Fig. 2, but for the small In–N atomic condensate model. The PDOS of one In atom, one of the nearest N atoms, and a pair of Ga and N atoms far away is given.

Table 4 Contribution to the electron wave function at the Γ point of the top valence band due to one In, N and Ga (far away In) atoms, respectively, in the wurtzite In₅Ga₃₁N₃₆ alloys with different In distributions.

configuration	uniform	chain	condensate
In	0.015	0.027	0.048
Ga	0.009	0.008	0.003
near N	0.018	0.036	0.063
far N	0.013	0.017	0.004

atoms and neighbouring N atoms, while the contribution of the other atoms is even less pronounced. The PDOS of the In 5p- and 4d-, especially the neighbouring N 2p-like states, have a spiculate peak at the VBM, and its band width is less than that of the chain model. All these facts clearly prove the characteristics of a stronger electron localization. The valence electrons with the highest energy are thus inclined to congregate in the vicinity of the In–N atomic condensate. Therefore, the In–N condensate can easily localize excitons to form radiative recombination centres, and the emission efficiency can be enhanced significantly.

In the electron wave function $\psi_{n,\mathbf{k}}(r)$, each *n* corresponds to an energy band, and each k denotes a k-point. In order to understand the electron localization better, we further focus on the characteristics of the electron wave function $\psi_{n,\mathbf{k}}(r)$ at the $k = \Gamma$ point of the top valence band in InGaN alloys. We present in Table 4 the site projected wave function character of $\psi_{n,\Gamma}(r)$, which is obtained by projecting the wave functions onto spherical harmonics of each atom. In the uniform model, all atoms have a definite contribution to the electron wave function $\psi_{n,\Gamma}(r)$ of the top valence band at the Γ point, and the highest possibility of a valence electron appearing around a atom (0.018) is only twice (0.009) of the lowest, which shows no electron localization in the VBM. In the chain model, the In and N atoms belong to the In-N-In atomic chain have a larger contribution to $\psi_{\Gamma}(r)$ than that of the other N and Ga atoms. Hence the electrons at VBM are localized around In-N-In atomic chains. In the atomic condensate model, we can see a strong electron localization in the vicinity of the small In-N atomic condensate due to a remarkable contribution of In (0.048) and the nearest N atom (0.063) to the electron wave function at the Γ point of the top valence band, which is 15 times higher than that of a Ga atom and N atom far away. Table 4 also clearly shows that the electron localization becomes much stronger than that in the chain model due to larger contribution of In and N (bonding with In) atoms. It is worth emphasizing that in terms of electron wave function projections the small In-N atomic condensate can strongly localize the valence electrons, which can be regarded as a radiative recombination centre of excitons. Hence the emission efficiency of InGaN alloys can be remarkably improved by these small In and N atomic condensates.

In order to help visually illustrate the nature of electron localization, we show in Fig. 4 the isosurfaces of the wave



Figure 4 (online colour at: www.pss-b.com) The isosurfaces of the wave functions of the HOMO-derived (VBM) bands $In_5Ga_{31}N_{36}$ alloys at the Γ point for the uniform model (a), chain model (b) and condensate model (c). In, Ga and N atoms are shown as red, grey and blue spheres, respectively. The 72-atom supercell is repeated along *x*-direction.

functions of the HOMO-derived (VBM) bands In₅Ga₃₁N₃₆ alloys at the Γ point for the uniform, chain and condensate models, respectively. The supercell is repeated along xdirection to clearly show the relations between In atoms. The spatial distribution of the wave function depends remarkably on the In distribution in the InGaN alloys. In the uniform model (Fig. 4a), the wave function distributes uniformly in space, and prefers to congregate in the comparative In-rich regions. In the chain model (Fig. 4b) and the condensate model (Fig. 4c), there is obvious electron localization along the In-N-In zigzag chains and in the In-N atomic condensates. This electron localization phenomenon is in great agreement with previous experiment proposed by Chichibu et al. [13]. It is noticeable that the high-value wave functions localize around the N atoms bonding with In atoms in all the three models, due to the contribution of the 2p-like states of the neighbouring N atoms based on the PDOS in Figs. 2 and 3.

3.3 Electron delocalization in AlGaN alloys We also perform the same calculations on the wurtzite $Al_5Ga_{31}N_{36}$ alloys with uniform and condensate configurations, and the distributing position of Al atoms in the two models are totally the same in characteristics as that of In

atoms in corresponding models. The calculations show that the total energy of the uniform model is a little lower than that of the cluster model (less than 0.1 eV). The calculated electronic structures of AlGaN alloys show direct bandgaps with the energies higher than those of InGaN alloys. The

electronic structures of AlGaN alloys show direct bandgaps with the energies higher than those of InGaN alloys. The bands in the VBM and CBM have obvious dispersion, and there is no defect level either in the valence band or conductive band. In order to compare with the best electron localization model in InGaN, we contrast the band width of the VBM band in these models. The values are 0.55 and 0.56 eV for the uniform model and condensate model, respectively, higher than the counterpart value (0.40 eV) in the InGaN condensate model. This shows that there is no strong electron localization in the VBM in AlGaN alloys. This fact is also validated by the PDOS calculation (not plotted here).

The calculation of the wave function $\psi_{n,\Gamma}(r)$ can further help to analyse the result. We show in Table 5 the site projected wave function character of VBM at the Γ point, and the character of $\psi_{n,\mathbf{k}}(r)$ at other k-points is similar to that of $\psi_{n,\Gamma}(r)$. The values are the possibilities of a valence electron appearing around some certain atoms of the alloys of various models. It is clear that unlike InGaN cluster model, in the AlGaN alloys, the contribution of the electron wave function around an Al atom to $\psi_{n,\Gamma}(r)$ is almost zero in both uniform model and condensate model. In the condensate model, the contribution of a Ga atom to $\psi_{n,\Gamma}(r)$ is higher than that in the perfect GaN, and the contribution of an N atom bonding with Al atoms is much lower than that of an N atom far away from the impurities. In the uniform model, all atoms make similar contribution to $\psi_{n,\Gamma}(r)$ compared with the perfect GaN model, except Al atoms. The results illuminate that there is slight delocalization phenomena near the Al atoms, which distinguishes from the InGaN alloy models. For the same concentration in the AlGaN and InGaN alloys, strong electron localization appears in the InGaN cluster configuration, not in the AlGaN models. Therefore, in the AlGaN alloys, excitons cannot be localized to form recombination centres that remarkably affect its internal quantum efficiency and PL emission efficiency. On the other hand, the valence electron localization in In-N condensates formed by chance in InGaN alloys can cause excitons to form recombination centres, and the emission efficiency can thus be improved by a long way.

Table 5 Characteristics of wave function $\psi_{n,\Gamma}(r)$ of different wurtzite (Al, In, Ga)N alloys. (u) and (c) denotes uniform model and condensate model, respectively, and the impurity row corresponds an aluminium atom, an indium atom or a gallium atom in the same position of different models.

alloy	AlGaN(u)	AlGaN(c)	InGaN(c)	GaN
impurity	0.001	0.001	0.048	0.010
Ga	0.010	0.015	0.003	0.010
near N	0.019	0.006	0.063	0.020
far N	0.021	0.033	0.004	0.020



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4 Conclusion In summary, the electronic structures of wurtzite (Al, In, Ga)N alloys are investigated by means of the first-principle calculations for InGaN in three models: the In distributed uniformly, the In-N-In chain and the small In-N atomic condensate models. Our total energy calculations show that the uniform model has the lowest energy, while both chain and condensate models can also form by chance at definite possibilities because of the small total energy differences (only 0.53 eV higher than the uniform model). In particular we know from the calculations of the electron PDOS and wave function at VBM that (1) the uniform model does not show any electron localization at VBM; (2) the valence electrons at VBM are localized weakly along the short In-N-In atomic chains and (3) the small In-N atomic condensates can localize the electrons strongly. It is this electron localization in the vicinity of the small In-N atomic condensates or the short In-N-In atomic chains that remarkably improve the emission efficiency of the InGaN alloys. The results of electron localization in AlGaN alloys show that the valence electrons prefer not to appear in any specific positions, and the AlGaN alloys obviously do not have advantage over InGaN alloys in aspects of the internal quantum and emission efficiency.

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