Quasiparticle self-consistent GW theory of III-V nitride semiconductors: Bands, gap bowing, and effective masses

A. Svane,[1] N. E. Christensen,[1] I. Gorczyca,[2] M. van Schilfgaarde,[3] A. N. Chantis,[4] and T. Kotani[5]
[1]*Department of Physics and Astronomy, Aarhus University, DK-8000 Aarhus C, Denmark*
[2]*High Pressure Research Center, Polish Academy of Sciences, Warsaw, Poland*
[3]*School of Materials, Arizona State University, Tempe, Arizona 85287-6006, USA*
[4]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[5]*Department of Applied Physics and Mathematics, Tottori University, Tottori 680-8552, Japan*
(Received 31 May 2010; published 1 September 2010)

The electronic band structures of InN, GaN, and a hypothetical ordered $InGaN_2$ compound, all in the wurtzite crystal structure, are calculated using the quasiparticle self-consistent GW approximation. This approach leads to band gaps which are significantly improved compared to gaps calculated on the basis of the local approximation to density functional theory, although generally overestimated by 0.2–0.3 eV in comparison with experimental gap values. Details of the electronic energies and the effective masses including their pressure dependence are compared with available experimental information. The band gap of $InGaN_2$ is considerably smaller than what would be expected by linear interpolation implying a significant band gap bowing in InGaN alloys.

DOI: 10.1103/PhysRevB.82.115102 PACS number(s): 71.20.Nr

I. INTRODUCTION

The nitride semiconductors AlN, GaN, and InN hold great potential for applications in optical devices. Their band gaps vary from 0.7 eV in InN to 3.5 eV in GaN and 6.2 eV for AlN, and by appropriate alloying, the range of available gap energies spans from the infrared to the ultraviolet. The progress in sample preparation techniques has recently led to a revision of the fundamental gap characteristics of InN. While previously the gap was found to be around 2 eV,[1–3] recent low temperature values are 0.61 eV,[4] 0.62 eV,[5] or 0.69 eV.[6,7] The InN conduction band has a rather peculiar form with a distinct nonparabolic shape and a low state density above the fundamental gap, which leads to a strong dependence of the spectral distribution of luminescence light on carrier concentration.[8] When InN is alloyed with GaN the fundamental gap increases, however a significant nonlinear dependence on Ga concentration (band gap bowing) is observed.[9]

Theoretical investigations of nitride semiconductors have usually started from the local approximation (LDA) to density-functional theory, which with great success describes the total energy aspects such as lattice constants, equation of state, and relaxations of atomic coordinates around defects and at surfaces. For the calculations of electronic excitation energies the LDA is less satisfactory, especially for the calculations of semiconductor band gaps. Often, the LDA band gaps are 50%–80% too small, in the case of InN even 100%, as the LDA band structure for InN is in fact metallic. To obtain reliable gaps in semiconductors additional modeling beyond LDA has to be added, e.g., most crudely the rigid "scissors operator" shift of unoccupied bands with respect to the occupied ones, the inclusion of *ad hoc* external potentials (LDA+C) approach,[10] or hybrid exchange functionals.[11] A more fundamental approach is offered by the GW approximation,[12] which is named after its construction of the electron self-energy from the Green's function (G) and the screened interaction (W) in the solid state environment. The proper inclusion of both dynamical and non-local effects by the GW approach leads to much improved band gaps compared to the LDA.[13] The GW approach depends on the band structure entering the evaluation of G and W. Often LDA band structures are used, as have been reported in several studies of wurtzite GaN and InN.[14–18] In contrast, Rinke *et al.*[19] used exact-exchange band structures as their input for GW calculations of GaN and InN, and Bechstedt *et al.*[20] used a hybrid screened exchange band structure for their GW calculation of wurtzite InN, as well as cubic GaN and InN. Common to all these studies is the confirmation that GW improves considerably the band gap of nitride semiconductors compared to LDA, while discrepancies in quantitative results most probably reflect details of the implementation of the GW approximation.

In this work we undertake an investigation of the InN and GaN band structure using the GW approximation in the newly developed quasiparticle self-consistent approach (QSGW),[21,22] which enforces as good accordance as possible between the input band structure entering the evaluations of G and W, and the calculated output GW band structure. The differences between the LDA and QSGW band structures are quantified, with emphasis on discussion of band gap, electron effective mass and the influence of hydrostatic pressure on these quantities. To investigate aspects of the bowing in InN-GaN alloys, also a fictitious $InGaN_2$ system in the wurtzite structure is investigated. For this system the LDA is used to optimize the structural parameters, and the QSGW to calculate the band structure at optimum structure. To correct for the slight overestimation of the band gaps calculated in the QSGW approximation, we have also applied an empirical hybrid approach,[23] which combines 80% of the QSGW self-energy with 20% of the LDA self-energy, and which leads to quite favorable merits when compared to experimental values of gaps and effective masses.

This paper is organized as follows: In Sec. II the QSGW methodology is briefly discussed and calculational details

presented. In section III the QSGW band structure results for GaN, InN, and $InGaN_2$ are presented and discussed. Finally, Sec. IV draws the conclusions of the present work.

II. METHODOLOGY

The GW approximation[12] is formally the first term in an expansion of the nonlocal and energy-dependent self-energy $\Sigma(\mathbf{r},\mathbf{r}',\omega)$ in the screened Coulomb interaction W. A more physically appealing picture views the GW as a dynamically screened Hartree-Fock approximation plus a Coulomb hole contribution.[12] The quasiparticle energies ϵ_α and wave functions $\psi_\alpha(\mathbf{r})$ are solutions to the equation

$$\hat{H}_0\psi_\alpha(\mathbf{r}) + \int \Sigma(\epsilon_\alpha,\mathbf{r},\mathbf{r}')\psi_\alpha(\mathbf{r}')d^3r' = \epsilon_\alpha\psi_\alpha(\mathbf{r}), \qquad (1)$$

where $\hat{H}_0$ is the Hamiltonian of a noninteracting reference system, and the self-energy operator Σ in GW is expressed as

$$\Sigma(\omega,\mathbf{r},\mathbf{r}') = \frac{i}{2\pi}\int G_0(\omega+\omega',\mathbf{r},\mathbf{r}')W(\omega',\mathbf{r},\mathbf{r}')d\omega'. \qquad (2)$$

In this equation G_0 is the Green function of the uncorrelated reference system, while W denotes the screened Coulomb interaction. Very often G_0 is constructed from a density functional based band structure (e.g., LDA), in which case the reference system strictly speaking is not uncorrelated, but the potential due to correlation is the exchange-correlation potential, V_{xc}, which is explicitly known and can be subtracted: $\Sigma \rightarrow \Sigma - V_{xc}\delta(\mathbf{r}-\mathbf{r}')$. The bare interaction between two electrons in positions $\mathbf{r}$ and $\mathbf{r}'$ is

$$v(\mathbf{r}-\mathbf{r}') = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}, \qquad (3)$$

where e denotes the electron charge. This interaction potential is screened by the presence of the other electrons in the solid, which is expressed through the dielectric function $\varepsilon(\omega,\mathbf{r},\mathbf{r}')$, so that the effective interaction is

$$W(\omega,\mathbf{r},\mathbf{r}') = \int \varepsilon^{-1}(\omega,\mathbf{r},\mathbf{r}'')v(\mathbf{r}''-\mathbf{r}')d^3r''. \qquad (4)$$

The dielectric function is calculated in the random phase approximation as $\varepsilon = 1 - vP$, where the polarization function P is given as $P = -iG_0 \times G_0$.

The above equations thus outline a mapping $\hat{H}_0 \rightarrow \Sigma$. However, from the self-energy operator an "optimum" nonlocal one-electron "exchange-correlation" potential may be constructed,[21,22] defining a mapping $\Sigma \rightarrow \hat{H}_0$. The combined mapping may therefore be iterated to self-consistency, and at self-consistency the reference system, described by $\hat{H}_0$, has a band structure as close as possible[22] to the true quasiparticle band structure in Eq. (1).

The GW approach neglects several contributions to the full self-energy operator, which can be collected as vertex corrections in the GW formalism.[12] Leading vertex corrections have been studied in a few cases,[24–26] but the computing effort is large. In the present work we apply the simpler empirical approach[23] of reducing the GW self-energy by a factor 0.8 to obtain good quantitative agreement with experimental gaps.

The electronic structure calculations were done with the linear muffin-tin orbital (LMTO) method[27] in the full-potential version of Ref. 28. Inside muffin-tin spheres, the orbitals are represented by angular sums of numerical radial functions. The orbitals are matched onto smoothed Hankel functions in the interstitial region. Two sets of orbitals, with *spdf* and *spd* characters, respectively, with different decay rates in the interstitial region, were used on each atomic site. Additional orbitals of *spd* character were placed on interstitial sites. the 3*d*- and 4*d*-semicore states of Ga and In were treated as part of the valence bands using local orbitals.[29] The tails of the orbitals were expanded inside other muffin-tin spheres with a cutoff of $\ell_{max}=4$. The self-energy was evaluated on an $8\times8\times6$ k-mesh. All scalar-relativistic effects are included in the QSGW self-consistency cycle. Spin-orbit coupling is, however, not included during the QSGW self-consistency iterations, but may be included as an extra term in the Hamiltonian for the final computation of quasiparticle band structure, which was however not considered here.

The wurtzite crystal structure is hexagonal, space group No. 186 ($P6_3mc$), with cations in positions (0,0,0) and $(a/\sqrt{3},0,c/2)$, and anion (N) in positions $(0,0,uc)$ and $[a/\sqrt{3},0,c(u-1/2)]$, where a and c are the two lattice constants, and u an additional internal configurational parameter. The $InGaN_2$ structure is modeled by placing In at (0,0,0), Ga at $(a/\sqrt{3},0,u_{Ga}c)$, and two N atoms at $(0,0,u_{N_\alpha}c)$ and $(a/\sqrt{3},0,u_{N_\beta}c)$ in the hexagonal cell, i.e., alternating layers of In and Ga. The symmetry is in this case lowered to $P3m1$, space group No. 156. Table I lists the structural data used in the present calculations. For GaN and InN the c/a ratio and u parameter were optimized at the experimental specific volume by LDA total energy calculations, while for $InGaN_2$ the volume was also determined by the global LDA total energy minimum. Alloys of GaN and InN are of considerable interest in the entire composition range for the tuning of luminescence properties, and these may be modeled by supercell calculations, as e.g., in Ref. 9, but the increased computational efforts of the QSGW approximation compared to LDA prohibits our investigation of larger unit cells.

III. RESULTS AND DISCUSSION

A. Band structures

The calculated self-consistent quasiparticle band structures of InN, GaN and $InGaN_2$ are presented in Figs. 1–3 and compared to their LDA counterparts. In all three cases the most significant feature to observe is the increasing gap between the valence and conduction bands within the QSGW approximation, which is a well-established general property of GW.[13] Furthermore, the QSGW approximation causes a significant shift of the semicore states (Ga 3*d* and In 4*d*, respectively) compared to LDA (not shown in the figures) as was discussed in Refs. 30 and 31. The In and Ga semicore *d*-states shift down with QSGW relative to LDA,

TABLE I. Lattice parameters a and c, in Å, and internal parameter, u, of GaN, InN and $InGaN_2$. The experimental data are room temperature data from a: Ref. 38 and b: Ref. 1. The lattice parameters obtained in theory are optimized (LDA) parameters *at the experimental volumes*. No experimental determination of the u parameter for InN has been published. For $InGaN_2$ three internal parameters are given, corresponding to the z-coordinate of the Ga, N_α, and N_β atoms relative to In (see text for discussion). The last row compares the theoretical equilibrium volumes (in $Å^3$ per formula unit) with the experimental volumes (for the binaries). As is most often the case the LDA equilibrium volumes are slightly lower than the experimental volumes.

	GaN		InN		$InGaN_2$
	Theory	Expt.[a]	Theory	Expt.[b]	Theory
a	3.189	3.190	3.543	3.544	3.335
c	5.196	5.189	5.721	5.718	5.482
c/a	1.630	1.627	1.615	1.613	1.644
u	0.3766	0.377	0.3793		0.4993
					0.1500
					−0.3940
V_{min}	22.34	22.86	30.21	31.10	26.40

[a]This work.
[b]LDA with gap correction, Ref. 8 and this work.

by 2.5–3.5 eV. Fuchs *et al.*[30] find that the d-binding energy for cubic GaN in self-consistent GW is 16.5 eV (relative to the valence band maximum), which compares favorably to the value 16.8 eV computed in the present work for wurtzite GaN. For cubic InN the same authors quote a (non-self-consistent) GW d-binding energy of 15.1–15.6 eV, the last digit depending on the underlying start band structure. Again, these results are in good accordance with the present (self-consistent) value of 15.7 eV for the wurtzite InN compound.

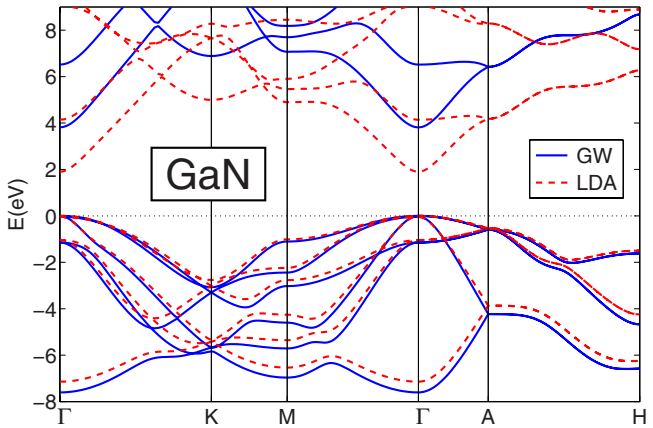

FIG. 1. (Color online) Comparison of QSGW (full line and blue) and LDA band structures (dashed line and red) of GaN. The zero of energy is placed at the valence band maximum. The calculation used the experimental parameters listed in Table I.

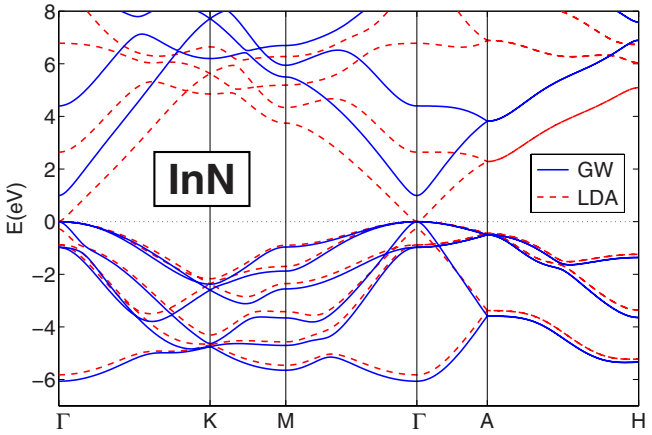

FIG. 2. (Color online) Comparison of QSGW (full line and blue) and LDA band structures (dashed line and red) of InN. The zero of energy is placed at the valence band maximum. The calculation used the experimental lattice parameters listed in Table I together with the theoretically determined u parameter.

The LDA value of the fundamental gap of InN is in fact negative, while those of $InGaN_2$ and GaN are 0.38 eV and 1.90 eV, respectively. Within the QSGW approximation, these gaps increase to 0.99, 1.80, and 3.81 eV, respectively, which for InN and GaN are considerably closer but slightly (0.2–0.3 eV) above the experimental band gaps. In all cases the minimum gap is direct and at the Γ point. Table II lists these numbers as well as other special point energies. Several effects contribute to the larger gap obtained by the QSGW theory compared to experiment: exciton interactions and other vertex corrections are not considered in theory, and the coupling to lattice vibration may also reduce the band gap.[32] In their self-consistent GW calculation of cubic GaN, Fuchs *et al.*[30] found a band gap of GaN of 3.53 eV, which similarly to the present calculation is ~0.3 eV larger than the experimental gap (3.20 eV). For the wurtzite structure, gaps of 3.32 eV[19] for GaN, and 0.72 eV[19] and 0.71 eV[20] for InN,

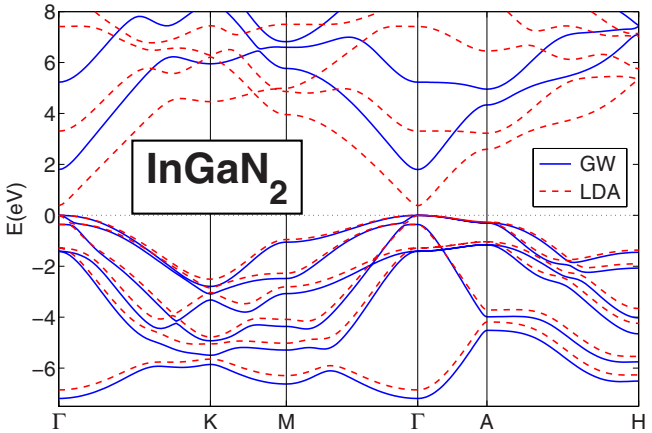

FIG. 3. (Color online) Comparison of QSGW (full line and blue) and LDA band structures (dashed line and red) of $InGaN_2$. The zero of energy is placed at the valence band maximum. The calculation used the theoretical parameters listed in Table I.

TABLE II. Minimum energy gap, $E_g(min)$, and N p-band width, $W(N_p)$, as calculated in quasiparticle self-consistent GW, LDA and the hybrid approach for GaN, InN, and $InGaN_2$. Also quoted are the position of semicore d states, $E(d)$ (defined as the average position of the semicore d levels at the Γ point), and the near-gap band energies at the K and M points, relative to the valence band maximum. Units are eV. The experimental gaps of GaN and InN are from: a: Ref. 39, b: Ref. 34, c: Ref. 4, d: Ref. 5, e: Refs. 7 and 6.

	GaN			InN			$InGaN_2$		
	QSGW	Hyb.	LDA	QSGW	Hyb.	LDA	QSGW	Hyb.	LDA
$E_g(min)$	3.81	3.42	1.90	0.99	0.74	−0.21	1.80	1.51	0.38
$E_g(exp)$		3.50[a], 3.51[b]			0.78,[b] 0.61[c]				
					0.62,[d] 0.69[e]				
$W(N_p)$	7.60	7.53	7.14	6.07	6.02	5.91	7.19	7.13	6.85
$E(d)$	−16.8	−16.2	−13.3	−15.7	−15.2	−13.1	−15.7	−15.4	−13.2
							−17.3	−16.6	−14.2
K_v	−3.07	−3.02	−2.76	−2.38	−2.33	−2.20	−2.79	−2.73	−2.50
K_c	6.89	6.49	5.00	6.20	5.92	4.83	5.95	5.65	4.46
M_v	−1.10	−1.07	−1.01	−0.96	−0.95	−0.91	−1.05	−1.03	−0.95
M_c	7.07	6.62	4.90	5.50	5.15	3.79	5.77	5.41	3.96

[a]This work.
[b]LDA with gap correction, Ref. 8 and this work.
[c]Reference 34.
[d]Reference 36.
[e]Reference 40.

were found in non-self-consistent GW calculations (based on two different flavors of screened exchange calculations). It is a general trend that invoking the self-consistency in the GW approximation leads to slightly too large gaps compared to experimental values,[23,30] and also to larger gaps than obtained in non-self-consistent calculations (with reasonable input band structure).[30] Other features of the band structures of GaN and InN to notice are that the width of the N p valence bands is slightly increased by .25–.45 eV in QSGW compared to LDA, and that the gap does not increase uniformly over the Brillouin zone. From the numbers in Table II it is evident that the gap increase in QSGW is up to 0.5 eV larger at the M point than at the Γ point. Hence, approximations based on rigid band shifts are inaccurate for these systems.

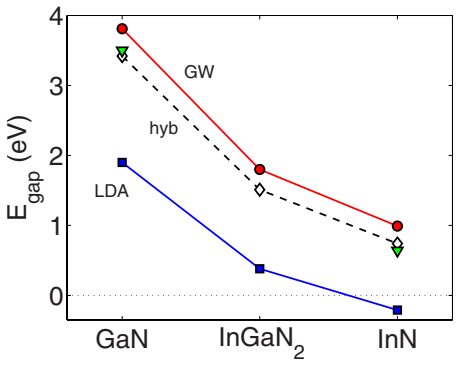

FIG. 4. (Color online) Comparison of QSGW (circles and red) and LDA (squares and blue) values of the fundamental energy gap (in eV) of wurtzite GaN, InN and $InGaN_2$. The experimental gaps of GaN and InN are also marked (triangles and green), and the dashed line marks the gaps calculated with the hybrid approach.

In Fig. 4 the fundamental gaps of GaN, InN, and $InGaN_2$ as calculated with LDA, QSGW and the hybrid approach, are compared. The experimental gaps of GaN and InN are likewise marked. The hybrid approach is indeed seen to give gaps very close to the experimental gaps, for which reason we will assume that also the remainder of the band structure is most accurately given by this approach, i.e., the neglect of vertex corrections inherent in the GW approach is well compensated by this 20% reduction of the self-energy operator. One notices a characteristic bowing: if the gap of the $InGaN_2$ compound is expressed in terms of the bowing parameter b as:

$$E_g(\mathrm{InGaN_2}) = 0.5[E_g(\mathrm{InN}) + E_g(\mathrm{GaN})] - 0.25b,$$

values of $b=2.40$ eV and $b=2.28$ eV are found in the QSGW and hybrid approaches, respectively. For comparison, with the LDA+C approach (LDA with empirical adjustment of bands[10]), a bowing parameter of =2.10 eV was found for $x=0.5$ for a supercell study of $In_xGa_{1-x}N$ alloys,[33] while experimental values of 1.4 eV (Ref. 34) and 1.37 eV (Ref. 35) have been found. The somewhat larger bowing found in the present calculations may reflect the fact that our $InGaN_2$ system is an ordered crystalline compound and not a random or quasirandom alloy as studied by experiment. On the other hand, the GW calculations of Ref. 17 (based on LDA band structures) imply a bowing of 1.44 eV, i.e., in very good agreement with the experimental value, even though the gaps of wurtzite GaN and InN (3.16 eV and 0.02 eV, respectively) in these calculations compare less favorably with the experi-

TABLE III. Effective electron masses for GaN, InN, and $InGaN_2$ in units of the free electron mass. $m_\perp$ and $m_\parallel$ denote the transverse and longitudinal masses corresponding to directions perpendicular and parallel to the hexagonal axis, respectively.

		Theory			
Compound		QSGW[a]	Hybr.[a]	LDA+C [b]	Expt.
GaN	$m_\perp$	0.204	0.201	0.28	0.20,[c] 0.237(6)[d]
	$m_\parallel$	0.182	0.179	0.26	0.20,[c] 0.228(8)[d]
InN	$m_\perp$	0.073	0.061	0.070	0.07,[c,e] 0.047,[f] 0.05[g]
	$m_\parallel$	0.066	0.058	0.068	0.07,[c,e] 0.039,[f] 0.05,[g] 0.085[h]
$InGaN_2$	$m_\perp$	0.129	0.122		
	$m_\parallel$	0.119	0.114		

[a]This work.
[b]LDA with gap correction, Ref. 8 and this work.
[c]Reference 34.
[d]Reference 36.
[e]Reference 40.
[f]Reference 37.
[g]Reference 41.
[h]Reference 42.

mental values. The gap calculated for $InGaN_2$ by these authors is 1.23 eV, i.e., somewhat smaller than that calculated in the present work (1.51 eV in the hybrid approach, cf. Table II).

B. Effective masses

In Table III are summarized the calculated effective masses of GaN, InN and $InGaN_2$ for the lowest conduction band. The QSGW electron masses are seen to be quite close to the experimental values, while the hybrid approach leads to a reduction of the effective electron masses compared to full QSGW. This reduction is rather small for GaN and $InGaN_2$ but significant for InN (~15%). The theoretical masses show a slight anisotropy, with the transverse masses (i.e., corresponding to directions in k-space perpendicular to the hexagonal axis) roughly 10% higher than the longitudinal masses (corresponding to k along the hexagonal axis). Most experimental values do not resolve any anisotropy, except for the infrared ellipsometry measurements on GaN in Ref. 36 and on InN in Ref. 37, which find ~4% and ~20% higher transverse effective masses, respectively.

C. Pressure effects

The pressure dependence of the band parameters are summarized in Table IV, which gives the calculated deformation potentials, γ, of the gaps at the zone center and at the K and M points, where

$$\gamma = \frac{d\epsilon}{d \ln V}.$$

These were calculated by varying the equilibrium volume by ±1% around the experimental volume (Table I) and including relaxation of the c/a ratio and u parameter as given within LDA. In all cases the gaps increase with compression, however at uneven rates: In GaN, the deformation potentials of the direct gaps at Γ, K, and M are −8.2, −4.0 and −5.4 eV, respectively, i.e., the gap at Γ increases most. In InN, on the other hand, the deformation potentials are −4.8, −4.4 and −7.5 eV at Γ, K, and M, i.e., in this case the gap at M increases fastest with compression. The calculated results are in excellent agreement with the available experimental results, not least for the pressure coefficients in view of the fact that the experiments are done on thin GaN epilayers on sapphire substrates.

TABLE IV. Deformation potentials for the band edge states closest to the gap at the Γ, K, and M points (in eV measured relatively to the valence band maximum). Also quoted are the deformation coefficients, $\kappa = d \ln m / d \ln V$, for the electron effective masses. These quantities were all evaluated at the experimental volume (Table I) using the hybrid approach, including the volume variation of the theoretically (LDA) optimized structural parameters, u and c/a. Experimental data are from a: Ref. 43, b: Ref. 9, c: Ref. 8.

	GaN	InN	$InGaN_2$
$\gamma(\Gamma_c)$	−8.2	−4.8	−3.5
$\gamma(\Gamma_c)$ (expt.)	−9.36(4)[a]	−4.0(4)[b]	
$\gamma(K_v)$	+3.3	+3.3	+3.7
$\gamma(K_c)$	−0.7	−1.1	−1.8
$\gamma(M_v)$	+1.3	+1.5	+1.2
$\gamma(M_c)$	−4.1	−6.0	−2.7
$\kappa(m_\perp)$	−1.8	−4.9	−1.2
$\kappa(m_\parallel)$	−1.9	−5.4	−1.5
$\kappa(m)$ (expt.)		−5.0[c]	

IV. CONCLUSION

The band structures of wurtzite InN and GaN and a fictitious $InGaN_2$ compound have been investigated with the quasiparticle self consistent GW approximation. Good accordance with available experimental information is found with this approach, which further facilitates a detailed investigation of effective masses and the effects of pressure on these. The QSGW calculations further show that for these materials corrections for the "LDA gap error" cannot be made by a rigid upwards shift of the conduction bands. Also the dispersion in the conduction bands is poorly described in the LDA bands.

ACKNOWLEDGMENTS

A.S. and N.E.C. acknowledge support from the Danish Center for Scientific Computing Center (DCSC) and the Danish Agency for Science, Technology and Innovation. M.v.S. was supported by NSF Grant No. QMHP-0802216.

[1] K. Osamura, S. Naka, and Y. Murakimi, J. Appl. Phys. **46**, 3432 (1975).
[2] V. A. Tyagai, A. M. Evstigneev, A. N. Krasiko, A. F. Adreeva, and V. Y. Malakhov, Sov. Phys. Semicond. **11**, 1257 (1977).
[3] T. L. Tansley and C. P. Foley, J. Appl. Phys. **59**, 3241 (1986).
[4] O. K. Semchinova, J. Aderhold, and J. Graul, Appl. Phys. Lett. **83**, 5440 (2003).
[5] J.-W. Yoon, S. S. Kim, H. Cheong, H.-C. Seo, S.-Y. Kwon, H.-J. Kim, Y. Shin, E. Yoon, and Y.-S. Park, Semi. Sci. Tech. **20**, 1068 (2005).
[6] J. Wu, W. Walukiewicz, W. Shan, K. M. Yu, J. W. Ager, S. X. Li, E. E. Haller, H. Lu, and W. J. Schaff, J. Appl. Phys. **94**, 4457 (2003).
[7] B. Arnaudov, T. Paskova, P. P. Paskov, B. Magnusson, E. Valcheva, B. Monemar, H. Lu, W. J. Schaff, H. Amano, and I. Akasaki, Phys. Rev. B **69**, 115216 (2004).
[8] I. Gorczyca, J. Plesiewicz, L. Dmowski, T. Suski, N. E. Christensen, A. Svane, C. S. Gallinat, G. Koblmueller, and J. S. Speck, J. Appl. Phys. **104**, 013704 (2008).
[9] G. Franssen, I. Gorczyca, T. Suski, A. Kaminska, J. Pereiro, E. Muñoz, E. Iliopoulos, A. Georgakilas, S. B. Che, Y. Ishitani, A. Yoshikawa, N. E. Christensen, and A. Svane, J. Appl. Phys. **103**, 033514 (2008).
[10] N. E. Christensen, Phys. Rev. B **30**, 5753 (1984).
[11] M. Marsman, J. Paier, A. Stroppa, and G. Kresse, J. Phys.: Condens. Matter **20**, 064201 (2008).
[12] L. Hedin and S. Lundqvist, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1969), Vol. 23, p. 1.
[13] M. S. Hybertsen and S. G. Louie, Phys. Rev. B **34**, 5390 (1986).
[14] M. Oshikiri and F. Aryasetiawan, J. Phys. Soc. Jpn. **69**, 2113 (2000).
[15] M. Oshikiri, F. Aryasetiawan, Y. Imanaka, and G. Kido, Phys. Rev. B **66**, 125204 (2002).
[16] D. Cociorva, W. G. Aulbur, and J. W. Wilkins, Solid State Commun. **124**, 63 (2002).
[17] M. Usuda, N. Hamada, K. Shiraishi, and A. Oshiyama, Jpn. J. Appl. Phys. **43**, L407 (2004).
[18] J. Furthmüller, P. H. Hahn, F. Fuchs, and F. Bechstedt, Phys. Rev. B **72**, 205106 (2005).
[19] P. Rinke, M. Scheffler, A. Qteish, M. Winkelnkemper, D. Bimberg, and J. Neugebauer, Appl. Phys. Lett. **89**, 161919 (2006).
[20] F. Bechstedt, F. Fuchs, and G. Kresse, Phys. Status Solidi B **246**, 1877 (2009).
[21] M. van Schilfgaarde, T. Kotani, and S. Faleev, Phys. Rev. Lett. **96**, 226402 (2006).
[22] T. Kotani, M. van Schilfgaarde, and S. V. Faleev, Phys. Rev. B **76**, 165106 (2007).
[23] A. N. Chantis, M. van Schilfgaarde, and T. Kotani, Phys. Rev. Lett. **96**, 086405 (2006).
[24] A. J. Morris, M. Stankovski, K. T. Delaney, P. Rinke, P. Garcia-Gonzalez, and R. W. Godby, Phys. Rev. B **76**, 155106 (2007).
[25] M. Shishkin, M. Marsman, and G. Kresse, Phys. Rev. Lett. **99**, 246403 (2007).
[26] N. E. Christensen, A. Svane, R. Laskowski, B. Palanivel, P. Modak, A. N. Chantis, M. van Schilfgaarde, and T. Kotani, Phys. Rev. B **81**, 045203 (2010).
[27] O. K. Andersen, Phys. Rev. B **12**, 3060 (1975).
[28] M. Methfessel, M. van Schilfgaarde, and R. A. Casali, in *Electronic Structure and Physical Processes of Solids*, Lecture Notes in Physics, edited by H. Dreysse (Springer-Verlag, Berlin, 2000), Vol. 535, p. 114.
[29] D. Singh, Phys. Rev. B **43**, 6388 (1991).
[30] F. Fuchs, J. Furthmüller, F. Bechstedt, M. Shishkin, and G. Kresse, Phys. Rev. B **76**, 115109 (2007).
[31] N. E. Christensen, I. Gorczyca, R. Laskowski, A. Svane, R. C. Albers, A. N. Chantis, T. Kotani, and M. van Schilfgaarde, Phys. Status Solidi B **246**, 570 (2009).
[32] M. Cardona and M. L. W. Thewalt, Rev. Mod. Phys. **77**, 1173 (2005).
[33] I. Gorczyca, S. P. Lepkowski, T. Suski, N. E. Christensen, and A. Svane, Phys. Rev. B **80**, 075202 (2009).
[34] I. Vurgaftman and J. R. Meyer, J. Appl. Phys. **94**, 3675 (2003).
[35] M. Marques, L. K. Teles, L. M. R. Scolfaro, J. R. Leite, J. Furthmüller, and F. Bechstedt, Appl. Phys. Lett. **83**, 890 (2003).
[36] A. Kasic, M. Schubert, S. Einfeldt, D. Hommel, and T. E. Tiwald, Phys. Rev. B **62**, 7365 (2000).
[37] T. Hofmann, T. Chavdarov, V. Darakchieva, H. Lu, W. J. Schaff, and M. Schubert, Phys. Status Solidi C **3**, 1854 (2006).
[38] H. Schulz and K. H. Thiemann, Solid State Commun. **23**, 815 (1977).
[39] B. Monemar, Phys. Rev. B **10**, 676 (1974).
[40] J. Wu, W. Walukiewicz, W. Shan, K. M. Yu, J. W. Ager, E. E. Haller, H. Lu, and W. J. Schaff, Phys. Rev. B **66**, 201403(R) (2002).
[41] S. P. Fu and Y. F. Chen, Appl. Phys. Lett. **85**, 1523 (2004).
[42] T. Inushima, M. Higashiwaki, and T. Matsui, Phys. Rev. B **68**, 235204 (2003).
[43] P. Perlin, L. Mattos, N. A. Shapiro, J. Kruger, W. S. Wong, T. Sands, N. W. Cheung, and E. R. Weber, J. Appl. Phys. **85**, 2385 (1999).