First-principles calculations of opto-electronic properties of IIAs (III = Al, Ga, In) under influence of spin–orbit interaction effects

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Abstract. In this article, we present first-principles calculations for structural and opto-electric properties of IIAs (III = Al, Ga, In) in the zinc-blende phase. Our calculations are based on the full potential-linearized augmented plane wave method implemented in the WIEN2k code. We employed Perdew–Burke–Ernzerhof generalized gradient and modified Becke–Johnson approximations as exchange–correlation potentials. Our calculated structure parameters are found to be in reasonable agreement with the available literature. It was found that the inclusion of spin–orbit interaction effect shifts the conduction band minima towards the Fermi level and provides band gaps very close to their experimental values. The optical properties such as complex dielectric functions, complex refractive indices, reflectivities, energy loss functions, optical conductivities and absorption coefficients at varied frequencies were investigated in detail. We found that static real part of dielectric functions and refractive index decreases with increase in band gap. Our calculated critical point energies (eV) are consistent with the experimental results.

Keywords. FP-LAPW; structural properties; electronic properties; spin–orbit interaction; optical properties.

1. Introduction

Group III–V semiconductors have significant importance due to their applications in optoelectronic operating systems from ultraviolet to the infrared range [1]. These compounds can produce novel materials having adjustable electronic as well as magnetic properties [2]. They crystallize in the zinc blende (ZB) and wurtzite phases [3]. But most of group III–V semiconductors exist in the ZB structure [4], within which the band gaps for III-arsenide (IIAs) always remain less than about 2.5 eV, and we can consider them as narrow band gap materials [5]. Due to this special property, IIAs compounds have been received extensive interest for their significant role in the semiconductor industry. These are specially valued for their applications in optoelectronic systems and devices such as solar cells, lasers and light-emitting diodes. Moreover, AlAs and GaAs owing to their specific characteristics are used in the formation of epitaxial multilayer structures such as hetero-junction bipolar transistors, high-electron mobility transistors and Bragg reflector superlattices including solid-state lasers [6]. GaAs, a direct band gap semiconductor material, has shown its promising and efficient role in photovoltaic systems. Overall, IIAs have a wide range of applications including the fabrication of photo-detectors, photodiodes, infrared-spectrum lasers, electro-optic modulators and frequency mixing components [7].

The electronic properties of IIAs have been studied in many experimental [8–13] and theoretical works [1,14–22]. Theoretically, different approaches have been used for calculations. These approaches include local density approximation (LDA) [1], Engel-Vosko generalized-gradient approximation (EV-GGA) [14], Tran Blaha modified Becke–Johnson (TB-MBJ) approximation [14–17], Perdew–Burke–Ernzerhof (PBE) approximation [17], local spin density approximation (LSDA) [18], Becke-3-Lee Yang Parr (B3LYP) approximation [18,23], Heyd–Scuseria–Ernzerhof (HSE) approximation [18,22], generalized density functional theory (GDFT) [19], Hartree–Fock approximation [20], MBJ +LDA [22] and Gowo approximation [1,21–23]. Most of these calculations are either based on semi-empirical techniques or simplified calculations that neglect some corrections like spin–orbit interaction (SOI) and orbit potential. The lack of these corrections makes the calculations easier and minimizes computational time, but the disadvantage is that the results do not match with the experimental results. IIAs (III = Al, Ga, In) compounds are not yet studied in the ZB phase using the full potential-linearized augmented plane wave (FP-LAPW) method with SOI. In order to explain the experimental results theoretically we studied the opto-electrical properties of these compounds with SOI. The addition of SOI provided all results close to experimental values as compared with other theoretical results.

2. Calculation method

The first-principles calculations of IIIAs (III = Al, Ga, In) were performed using the FP-LAPW method implemented in the WIEN2k code [24]. In this approach, the crystal unit cell is divided into two portions. The first portion consists of non-overlapping atomic spheres which are known as Muffin Tin (MT) spheres and the second portion is interstitial region. In the two regions, the wave functions, potentials and charge density are treated differently. For our calculations, GGA of PBE [25] and MBJ potential of Tran and Blaha [26] were employed as exchange–correlation potentials. For calculation of opto-electronic properties the effect of SOI was added which uses second variational strategy to improve the results [27]. To avoid the leakage of charge from the core, the MT radii for Ga, In, Al and As were taken as 2.3, 2.48, 2.32 and 2.31 Bohr, respectively. To expand the charge density as well as the potential, the maximum angular momentum $l_{\max} = 10$ was used inside the atomic spheres. To obtain the suitable total energy of convergence in interstitial region, a cut-off value of $k_{\max} = 7.0/R_{\text{MT}}$ was used. The charge density was restricted to 12 (Ryd) $^{1/2}$. A mesh of 1000 and 400k points in the first Brillouin zone was utilized for computation of structural and electronic properties, respectively.

3. Results and discussion

3.1 Structural properties

The ZB structure of IIIAs (III = Al, Ga, In) has a face-centred cubic lattice in which the position of group III element is (0, 0, 0) and position of As is (0.25, 0.25, 0.25) as shown in figure 1. In our study the ground-state properties of these compounds were calculated by an optimization process in which volume is varied and energy of each volume was calculated. The ground-state volume is that one which has minimum energy. Optimized volume of unit cell was obtained by plotting the unit cell volume against total energy and using the Birch Muraghan's equation of state [28,29]:

$$E(V) = E_0 + 9 \frac{V_0 B_0}{16} \left[\left\{ \left(\frac{V_0}{V} \right) - 1 \right\} B'_0 + \left\{ \left(\frac{V_0}{V} \right)^{2/3} - 1 \right\}^2 \left\{ 6 - 4 \left(\frac{V_0}{V} \right) \right\}^{2/3} \right]. \quad (1)$$

The optimized plots are given in figure 2. The ground-state lattice parameter a , bulk modulus B and bulk modulus pressure derivative B' were calculated from optimized volume. The ground-state parameters along with other calculated experimental and theoretical values are listed in table 1. Our calculated values are in good agreement with experimental values. Furthermore, in the periodic table down group III, it is observed that the lattice constant increases due to increase in atomic number while the bulk modulus decreases.

Figure 1. ZB structure of IIIAs.

Figure 2. Calculated energy vs. volume plots for AlAs, GaAs and InAs.

3.2 Electronic properties

The electronic density of states (DOS) and band structures were calculated with and without inclusion of SOI effect using MBJ potential approximation and are shown in figures 3–8. DOS gives information about the contribution of electronic states in different energy levels and rough idea of the band gap of a material. Figures 3–5 show the calculated total DOSs (TDOS) of IIIAs (III = Al, Ga, In) compounds without and with the addition of SOI and partial DOSs (PDOS) with SOI.

Table 1. Calculated ground-state lattice parameters a (Å), bulk modulus B (GPa), bulk modulus and pressure derivative B' (GPa) along with experimental and other simulated results.

Compounds		Present	Experimental	Others
AlAs	a	5.63	5.620 ^b , 5.661 ^c	5.614 ^d (PP-LDA), 5.690 ^m (PP-GGA), 5.664 ^h (FP-LDA), 5.644 ^p (FP-LDA), 5.741 ^f (HF), 5.76 ^q (HF)
	V	301.76		
	B	75.56	82.0 ^e , 77.3 ^a	74.7 ^d (PP-LDA), 71.0 ^m (PP-GGA), 71.0 ^h (FP-LDA), 75.4 ^p (PF-LDA), 90.0 ^f (HF), 79.0 ^q (HF)
	B'	4.13	4.182 ^e	4.182 ^d (PP-LDA), 4.4 ^p (HF)
GaAs	a	5.655	5.654 ^a , 5.653 ^k	5.651 ^h (FP-LDA), 5.530 ^d (PP-LDA), 5.700 ^m (PP-GGA), 5.508 ⁱ (FP-LDA), 5.726 ^j (FP-GGA), 5.755 ^f (HF)
	V	305.19		
	B	68.1766	77.0 ^e , 76.0 ^k	75.7 ^d (PP-LDA), 65.0 ^m (PP-GGA), 63.0 ^h (FP-LDA), 77.1 ⁱ (FP-LDA), 87.0 ^f (HF), 68.0 ^j (FP-GGA)
	B'	4.47	4.487 ^e	4.487 ^d (PP-LDA), 4.8 ^p (FP-LDA), 4.46 ^j (FP-LDA)
InAs	a	6.1	6.036 ^b	5.921 ^d (PP-LDA), 5.902 ^g (PP-LDA), 6.015 ^p (FP-LDA), 6.152 ^f (HF), 6.15 ^q (HF)
	V	398.73		
	B	52.58	58.0 ^e	61.7 ^d (PP-LDA), 61.9 ^g (PP-LDA), 60.3 ^p (FP-LDA), 74.0 ^f (HF), 64.0 ^q (HF)
	B'	4.75	4.79 ⁿ	4.545 ^d (PP-LDA), 4.488 ^g (PP-LDA), 4.9 ^p (FP-LDA)

^aRef. [3], ^bref. [30], ^cref. [9], ^dref. [31], ^eref. [32], ^fref. [33], ^gref. [34], ^href. [35], ⁱref. [36], ^jref. [37], ^kref. [38], ^lref. [39], ^mref. [40], ⁿref. [41], ^oref. [42], ^pref. [43], ^qref. [44].

Figure 3. DOS of AlAs: (a) comparison between the total DOS with and without SOI and (b) total and partial DOS with SOI.

Panel (a) of figures shows comparison between the TDOS with and without SOI, from which it can be deduced that DOS can be divided into four major peaks. The first three peaks contribute to the valence band (VB) and the fourth peak lies to the right side of the Fermi level and contributes to the conduction band (CB) maximum. When SOI is applied, a shift in the fourth peak is observed towards the Fermi level which reduces the forbidden energy gap. The electronic transitions actually occur between the maximum of VB and the minimum of CB, therefore, shift of the fourth peak is more significant as compared with other peaks. The reason of shifting can be explained as follows. In the electron's frame of reference the nucleus can be treated as making a current loop

Figure 4. DOS of GaAs: (a) comparison between the total DOS with and without SOI and (b) total and partial DOS with SOI.

around the electron. Thus electrons exist in the magnetic field of the current loop. The spin magnetic moment interacts with the magnetic field established by the orbital motion of the nucleus which results in the removal of degeneracy and splits the energy states [27]. The resulting states repel each other and reduces band gap.

Panel (b) in figures 3–5 shows the contribution of sub-energy levels to TDOS of AlAs, GaAs and InAs, respectively. Panel (b) of all figures shows that VB minimum has major contribution of s state of As and have minor contribution of s and p states of group III elements along with p state of As. VB maximum is majorly composed of p states of As along with minor contribution of s and p states of group III elements and s state of As. In the CB maximum the s state of group III elements has greater contribution and p state of group III elements along with s and p state of As has minor contribution while the CB minimum is mainly made of p state of group III elements along with minor contribution of s state of group III elements and s and p states of As.

The DOS plots give us the general idea of the band gap. However, to know the exact nature of band gap, we have to find variations of different energy levels along with symmetry points in the first Brillion zone. The calculated electronic band structures without and with SOI are shown in figures 6–8. The VB maximum and CB minimum lies at the same symmetry point Γ for GaAs and InAs, while the VB maxima for AlAs lies at Γ point and CB minima lies at X point. Hence, the fundamental band gap of GaAs and InAs is direct and AlAs is indirect. Our simulated band gaps along with other theoretical and experimental results are given in table 2. Our calculated

Figure 5. DOS of InAs: (a) comparison between the total DOS with and without SOI and (b) total and partial DOS with SOI.

Figure 6. Band gap of AlAs: (a) without SOI and (b) with SOI.

results are much closer to experimental results as compared with other previously published simulated results. The addition of SOI causes the splitting of As-p states at symmetry points W, L, X and Γ in the upper VB and the splitting of Al-s, Ga-s and In-s states at symmetry points L, Γ and W in the lower CB for AlAs, GaAs and InAs, respectively. This splitting causes repulsion between energy states which results in the shifting of Al-s states along the X point, and Ga-s and In-s states along the Γ point towards lower energy states. Due to splitting and shifting, reduced band gaps of all studied compounds were obtained, which lie within the experimental range.

3.3 Optical properties

The optical properties of IIIs (III = Al, Ga, In) were calculated using MBJ approximation with effect of SOI. The results were obtained without applying any broadening or scissor operators often employed to match theoretical calculations with experimental results [27]. The calculated optical spectral critical points along with other theoretical and experimental results are shown in table 3. Our calculated values

are in excellent agreement with experimental results and are better than other calculated results.

3.3a Dielectric function: The dielectric function $\varepsilon(\omega)$ describes the optical response to all photon energies and is given by [48]

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega). \quad (2)$$

The real part $\varepsilon_1(\omega)$ shows dispersive behaviour and imaginary part $\varepsilon_2(\omega)$ shows absorptive behaviour of the material. The real and imaginary parts of dielectric function up to 12 eV energy are plotted in figure 9a. The calculated zero-frequency limit, $\varepsilon_1(0)$ of AlAs, GaAs and InAs are 6.16, 9.14 and 9.54, respectively, which show that $\varepsilon_1(0)$ increases, when III goes down in the group of the periodic table from Al to In. Keeping this special behaviour and table 2 in mind, we can conclude that $\varepsilon_1(0)$ varies inversely with band gap for these materials. A similar behaviour was also discussed in other materials [49,50]. Beyond zero frequency limits, $\varepsilon_1(\omega)$ increases to maximum value 13.21 for AlAs, 15.02 for GaAs and 15.13 for InAs at their respective peak E_1 . After maximum peaks,

Figure 7. Band gap of GaAs: (a) without SOI and (b) with SOI.

$\varepsilon_1(\omega)$ decreases sharply below zero to the minimum value of -2.7 for AlAs, -4.9 for GaAs and -5.1 for InAs. For these negative values of $\varepsilon_1(\omega)$, the compounds lose dielectric property and show metallic character [51,52]. $\varepsilon_2(\omega)$ is related to the band gap of a material. Hence, for all three compounds, $\varepsilon_2(\omega)$ starts at our calculated band gap E_0 and increase with increase in energy. The maximum value of $\varepsilon_2(\omega)$ occurs at peak E_2 and then reaches zero by passing through another peak E_3 . For AlAs, GaAs and InAs, the calculated maximum values of $\varepsilon_2(\omega)$ are 18.37, 15.89 and 13.86, respectively.

3.3b Complex refractive index: The complex refractive index $\tilde{n}(\omega)$ is related to refraction and absorption of light by a material and is given by [48]

$$\tilde{n}(\omega) = n(\omega) + iK(\omega). \quad (3)$$

The real part $n(\omega)$ is called the refractive index shown by the solid line and imaginary part $K(\omega)$ is called the extinction coefficient shown by the dashed line in figure 9b. The value of the refractive index starts at zero frequency having a value of 2.46 for AlAs, 2.80 for GaAs and 3.07 for InAs.

The refractive index shows a similar behaviour to $\varepsilon_1(\omega)$, the value of $n(0)$ decreases with increase of band gap of these compounds. Beyond $n(0)$ limit, the value of $n(\omega)$ increases and reaches the maximum value of 3.93 for AlAs, 3.965 for GaAs and 4.00 for InAs, at their first peak E_1 . After maximum value, $n(\omega)$ decreases rapidly near E_2 and approaches to minimum values for higher energies. The extinction coefficient $K(\omega)$ shows similar behaviour to $\varepsilon_2(\omega)$.

3.3c Optical conductivity: When light of specific frequency falls on a material, conduction of electrons occurs. This property of a material is called optical conductivity $\sigma(\omega)$ and is given by [48]

$$\sigma(\omega) = \frac{2W_{cv}\hbar\omega}{E_0^2} \quad (4)$$

where W_{cv} is the transition probability per unit time.

The simulated plots of optical conductivity vs. incident photon energy with the effect of SOI are given in figure 10a. The optical conductivity $\sigma(\omega)$ like absorption coefficient for AlAs, GaAs and InAs starts at fundamental band gaps and

Figure 8. Band gap of InAs: (a) without SOI and (b) with SOI.

then increases at E_1 then sharply increases at E_2 and then decreases at E_3 . The maximum optical conductivity ranges for investigated compounds IIAs (III = Al, Ga, In) are 4.65–5.602, 4.48–5.06 and 4.05–4.86, respectively. In the maximum conductivity ranges these materials can be best utilized in solar cells and detectors in the ultra-violet energy range. $\sigma(\omega)$ has maximum value of $1.1795 \times 10^4 \Omega^{-1} \text{ cm}^{-1}$ for AlAs at E_2 , $1.0007 \times 10^4 \Omega^{-1} \text{ cm}^{-1}$ for GaAs at E_2 and $8.385 \times 10^3 \Omega^{-1} \text{ cm}^{-1}$ for InAs at the second peak.

3.3d Absorption coefficient: The absorption coefficient is the property of material to absorb photons of specific energy and is given by [48]

$$\alpha(\omega) = \frac{4\pi K(\omega)}{\lambda}. \quad (5)$$

The absorption coefficient calculated with SOI is shown in figure 10b. The figure shows that absorption for all of our studied compounds starts at their fundamental band gaps. While at peak E_1 the transition from As-p states in the VB to Al-s, Ga-s and In-s states in the CB of AlAs, GaAs and InAs, respectively, occurs which is designated as $L_{6,7}^V \rightarrow L_7^C$. The second peak E_2 for AlAs, GaAs and InAs corresponds to

maximum absorption $144.6 \times 10^4 \text{ cm}^{-1}$, $165.4 \times 10^4 \text{ cm}^{-1}$ and $162.3 \times 10^4 \text{ cm}^{-1}$, respectively, which shows transition $X_{6,7}^V \rightarrow X_7^C$ and the third peak E_3 for all studied compounds corresponds to transition $W_{6,7}^V \rightarrow W_7^C$.

3.3e Reflectivity: The reflection of incident light from the surface of a material corresponds to reflectivity and is given by [48]

$$R(\omega) = \left(\frac{|1 - n(\omega)|}{|1 + n(\omega)|} \right)^2. \quad (6)$$

The reflectivity $R(\omega)$ is plotted against the incident photon energy with addition of SOI in figure 10c. At zero frequency the reflectivity is called static reflectivity $R(0)$ having the value of 17.9% for AlAs, 22.6% for GaAs and 26.1% for InAs. In figure 10c the different peaks show variation in reflectivity when the energy increases. The maximum value of reflectivity for AlAs is 53% at 11.058 eV, GaAs is 61.2% at 11.93 eV and for InAs is 60.7% at 10.582 eV. It is observed that the maximum value of reflectivity occurs at point where $\varepsilon_1(\omega)$ becomes negative because in this energy range the material shows a metallic character [53].

Table 2. Fundamental band gaps in eV calculated without and with SOI for GaAs and InAs compared with previously calculated works and experimental values.

Compounds	Present		Experimental	Other theoretical works
	Without SOI	With SOI		
AlAs	2.32	2.23	2.24 ^a , 2.32 ^b , 2.3 ^c	1.31 ^a (LDA), 1.40 ^b (GGA), 2.25 ^c (EV-GGA), 1.98 ^d (MBJ) 2.12 ^c (TB-MBJ), 2.25 ^c (nTB-MBJ) 2.06 ^d (MBJ), 2.12 ^d (MBJ + PBE) 2.71 ^e (B3LYP), 2.24 ^e (HSE) 1.40 ^e (LSDA), 2.54 ^g (LDA) 1.58 ^g (GW), 2.73 ^h (GW) 2.48 ⁱ (LDA), 3.26 ^k (GW) 2.29 ^k (LDA), 3.3 ^l (B3LYP) 2.24 ^l (HSE)
GaAs	1.61	1.52	1.42 ^a , 1.52 ^b	0.28 ^a (LDA), 0.25 ^a (GGA) 1.03 ^a (EV-GGA), 1.56 ^b (MBJ) 1.6 ^c (TB-MBJ), 1.51 ^c (nTB-MBJ) 1.55 ^d (MBJ), 1.44 ^d (MBJ + PBE) 1.44 ^e (B3LYP), 1.21 ^e (HSE) 0.43 ^e (LSDA), 1.06 ^f (LDA) 1.58 ^f (GW), 1.60 ⁱ (LDA) 1.33 ^j (HSE06), 1.56 ^j (MBJLDA) 0.43 ^j (PBE), 1.47 ^k (GW) 0.56 ^k (LDA), 1.91 ^l (B3LYP) 1.21 ^l (HSE)
InAs	0.56	0.47	0.42 ^a , 0.42 ^b	0.00 ^a (LDA), 0.00 ^a (GGA) 0.40 ^a (EV-GGA), 0.60 ^b (MBJ) 0.66 ^c (TB-MBJ), 0.42 ^c (nTB-MBJ) 0.57 ^d (MBJ), 0.46 ^d (MBJ + PBE) 0.55 ^e (B3LYP), 0.39 ^e (HSE) 0.00 ^e (LSDA), 0.25 ^g (LDA) 0.31 ^g (GW), 0.46 ^h (GW) 0.42 ^j (HSE06), 0.61 ^j (MBJLDA) −0.30 ^j (PBE)

^aRef. [14], ^bref. [15], ^cref. [16], ^dref. [18], ^eref. [19], ^fref. [45], ^gref. [19], ^href. [21], ⁱref. [1], ^jref. [22], ^kref. [23], ^lref. [20].

From the reflectivity curves the three minima for AlAs occurs at 6.28, 8.25 and 9.48 eV, for GaAs occurs at 5.58, 6.92 and 8.88 eV and for InAs occurs at 5.24, 7.91 and 9.59 eV. These minima are related to transmission resonance frequencies.

3.3f Energy loss spectrum: The resonance of plasma is related to energy loss function which corresponds to the frequency of incident radiation. The energy loss function vs. incident light for AlAs, GaAs and InAs with addition of SOI is plotted in figure 10d. The plots show three peaks for AlAs at 6.28, 8.25 and 9.48 eV corresponding to frequencies 1.51×10^{15} , 1.99×10^{15} and 2.28×10^{15} Hz, three peaks for GaAs at energy 5.58, 6.92 and 8.88 eV corresponding to frequencies 1.34×10^{15} , 1.66×10^{15} and 2.14×10^{15} Hz and three peaks for InAs at 5.24, 7.91 and 9.59 eV corresponding to frequencies 1.26×10^{15} , 1.90×10^{15} and 2.31×10^{15} Hz, respectively. Above these frequencies the transmittance of

Table 3. Comparison of calculated and experimental values of characteristic peaks in optical spectra in eV.

Compounds	Peaks	This work	Other works	Experimental
AlAs	E ₁	4.3	3.5 ^a , 4.05 ^f	3.8 ^g , 3.90 ^g
	E ₂	4.78	4.4 ^a , 5.03 ^f	4.85 ^g , 4.89 ^g
	E ₃	5.81		
GaAs	E ₁	3.06	2.9 ^a , 3.16 ^b	3.017 ^c , 2.90 ^d
	E ₂	4.72	4.4 ^a , 4.83 ^b	5.11 ^c , 4.75 ^d
	E ₃	6.11		
InAs	E ₁	2.55	2.6 ^a	2.5 ^d , 2.6 ^e
	E ₂	4.45	4.3 ^a	4.45 ^d , 4.3 ^e
	E ₃	5.78		

^aRef. [8], ^bref. [46], ^cref. [12], ^dref. [9], ^eref. [13], ^fref. [47], ^gref. [11].

materials increases and shows transparent behaviour [54] because the maxima of energy loss function corresponds to minima of reflectivity.

Figure 9. (a) Dielectric function and (b) refractive index for AlAs, GaAs and InAs.

Figure 10. (a) optical conductivity, (b) optical absorption, (c) reflectivity and (d) energy loss spectrum for AlAs, GaAs and InAs.

4. Conclusions

In this study, we calculated the structural, electronic and optical properties of IIAs (II = Ga, In, Al) using the WIEN2k code based on DFT. For calculation of electronic and optical properties the SOI effect was included. The calculated ground-state properties are in good agreement with experiment. It was noted that when group III element changes from Al to In, the lattice parameters and derivative of bulk modulus increases while bulk modulus decreases. SOI effect breaks the degeneracy and splits the electronic states. The repulsion between the resulting states shifts CB minima towards the Fermi level, due to which reduced band gaps of AlAs

(Γ -X), GaAs (Γ - Γ) and InAs (Γ - Γ) were obtained which are comparable with experimental results. The static real part of complex dielectric function and refractive index decreases as band gap increases. Optical conductivity decreases by going from Al to In. Maxima of energy loss function corresponds to minima of reflectivity and in such situation IIAs compounds show transparent behaviour. From the optical spectra analysis these materials are predicted to be useful for optical applications in the infrared, visible and ultraviolet energy ranges.

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