

## Band Gap and Band Offset of $\text{Ga}_2\text{O}_3$ and $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ Alloys

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$\text{Ga}_2\text{O}_3$  and  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloys are promising materials for solar-blind UV photodetectors and high-power transistors. Basic key parameters in the device design, such as band-gap variation with alloy composition and band offset between  $\text{Ga}_2\text{O}_3$  and  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ , are yet to be established. Using density-functional theory with the Heyd-Scuseria-Ernzerhof hybrid functional, we compute formation enthalpies, band gaps, and band-edge positions of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloys in the monoclinic ( $\beta$ ) and corundum ( $\alpha$ ) phases. We find the formation enthalpies of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloys are significantly lower than that of  $(\text{In}_x\text{Ga}_{1-x})_2\text{O}_3$ , and that  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  with  $x = 0.5$  can be considered as an ordered compound  $\text{AlGaO}_3$  in the monoclinic phase, with Al occupying the octahedral sites and Ga occupying the tetrahedral sites. The band gaps of the alloys range from 4.69 to 7.03 eV for  $\beta$ - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  and from 5.26 to 8.56 eV for  $\alpha$ - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ . Most of the band offset of the  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloy arises from the discontinuity in the conduction band. Our results are used to explain the available experimental data, and consequences for designing MODFETs based on  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3/\text{Ga}_2\text{O}_3$  are discussed.

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$\text{Ga}_2\text{O}_3$  has been intensively investigated as a wide-band-gap semiconductor for high-power electronics [1–3] and UV solar-blind photodetectors [4,5]. It is available as large single crystals [6] suitable for high-quality epitaxial thin-film growth by metalorganic chemical vapor deposition (MOCVD) [7,8] and molecular beam epitaxy (MBE) [5,9]; it displays high breakdown electric field [1], and the Baliga figure of merit exceeds that of SiC and GaN [3]; it can be easily doped  $n$ -type, and band-gap engineering can be accomplished by incorporating In and Al, adding great flexibility to device design. Modulation doping of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3/\text{Ga}_2\text{O}_3$  heterostructures can be used to separate the ionized donors in the  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  layer from the conduction electrons in the  $\text{Ga}_2\text{O}_3$  layer [10–13], providing a boost to the electron mobility to about  $500 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  [10,14,15] by suppressing scattering from the ionized impurities. Simulated band diagrams and a 2DEG profile of MODFETs based on  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3/\text{Ga}_2\text{O}_3$  assumed that the discontinuity in the band offset appears solely on the conduction band [10]. However, this assumption has not been based on firm experimental evidence or first-principles calculations. The band gap of the  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloy and the band offset between the  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  and  $\text{Ga}_2\text{O}_3$  are key parameters in the device design and are yet to be established.

$\text{Ga}_2\text{O}_3$  and  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  can be made in the monoclinic ( $\beta$ ) and in the corundum ( $\alpha$ ) phase, as shown

in Fig. 1. Bulk and thin films of  $\beta$ - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  have been obtained using solution combustion synthesis [16], pulsed laser deposition (PLD) [17], and oxygen plasma-assisted MBE [10–12], while  $\alpha$ - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  have been grown on sapphire substrates by CVD for Al content of up to 81% [18,19]. Band gaps of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  for selected Al content have been reported [16–20], but band offsets between  $\text{Ga}_2\text{O}_3$  and  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ , which are much more challenging to obtain experimentally, are still unknown.

Using density functional theory (DFT) and the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional, we investigate the formability of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloys in both  $\beta$  and  $\alpha$  phases, their band gaps as a function of Al concentration, and the band offsets of the  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloys with respect to  $\text{Ga}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3$ . In the following, we first describe the details of the calculations, present the results for structural parameters and stability of the alloys, and then discuss the results for band gaps and band offsets for both  $\beta$  and  $\alpha$  phases and the implications for device design.

The calculations are based on DFT [33,34] with the projector augmented wave (PAW) method [35] as implemented in the VASP code [36,37]. The  $d$  states of Ga are included as valence states, and a plane-wave cutoff energy of 400 eV is employed. We use the Perdew-Burke-Ernzerhof functional revised for solids (PBEsol) [38] to relax all structures. To overcome the severe underestimation of band gaps in the DFT PBEsol functional, we employ the screened hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE06) [39,40]. In the HSE hybrid

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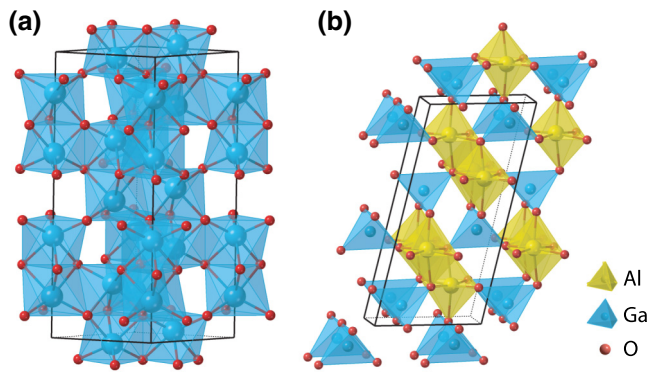


FIG. 1. Conventional unit cells of (a)  $\alpha$ - $\text{Ga}_2\text{O}_3$  and (b)  $\beta$ - $\text{AlGaO}_3$  compounds. In the latter, the Al atoms occupy octahedral sites and Ga occupy tetrahedral sites, maintaining the same structure as its parent compounds  $\beta$ - $\text{Ga}_2\text{O}_3$  and  $\theta$ - $\text{Al}_2\text{O}_3$ .

functional, the nonlocal Hartree-Fock exchange is mixed with the generalized gradient approximation (GGA) [41] exchange in the short-range part. The mixing parameter in HSE is fixed to 32% for all the calculations. We find that this choice of mixing parameter gives band gaps of the parent compounds  $\text{Ga}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3$  in good agreement with experimental values. Note that, conventionally, monoclinic  $\text{Al}_2\text{O}_3$  is often denoted as the  $\theta$  phase in the literature, i.e.,  $\theta$ - $\text{Al}_2\text{O}_3$  shares the same crystal structure as  $\beta$ - $\text{Ga}_2\text{O}_3$  [21–23]. The calculated lattice parameters, formation enthalpies, and band gaps for  $\text{Al}_2\text{O}_3$  and  $\text{Ga}_2\text{O}_3$  are listed in Table I along with the available experimental

data. The  $\theta$ - $\text{Al}_2\text{O}_3$ ,  $\alpha$ - $\text{Ga}_2\text{O}_3$ , and  $\beta$ - $\text{Ga}_2\text{O}_3$  have indirect gaps where the valence-band maximum is higher than the valence-band edge at  $\Gamma$  by 0.16, 0.24, and 0.04 eV, respectively, as previously reported [42].

We simulate  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  random alloys using special quasirandom structures (SQS) [43] generated using the mcsqs code of the Alloy Theoretic Automated Toolkit (ATAT) [44]. This method can generate optimal periodic supercells comparable to true disordered structures based on a Monte Carlo simulated annealing loop with an objective function that seeks to perfectly match the maximum number of correlation functions [44].

We use supercells containing 80 atoms for the  $\alpha$  and 120 atoms for the  $\beta$  phase. In the case of  $\alpha$ - $\text{Ga}_2\text{O}_3$ , all Ga sites are equivalent; therefore, Al tends to replace Ga randomly. However, in the case of  $\beta$ - $\text{Ga}_2\text{O}_3$ , half of the Ga atoms are at octahedral sites and the other half at tetrahedral sites. We find that Al strongly prefers octahedral sites, i.e., Al sitting at octahedral sites is approximately 0.2 eV per Al atom lower in energy than Al sitting at tetrahedral sites. Therefore, in the generation of SQS structures to simulate  $\beta$ - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloys, we assumed that Al atoms occupy only octahedral sites for  $x \leq 0.5$ . For  $x > 0.5$ , Al atoms exceeding  $x > 0.5$  randomly replace Ga at tetrahedral sites since all octahedral sites are already filled.

Figure 2 shows the calculated equilibrium volume of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloys as a function of Al fraction. For  $\alpha$ - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ , the volume varies linearly with Al composition, following Vegard’s law. For  $\beta$ - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ , the volume also decreases monotonically with Al fraction, but

TABLE I. Calculated lattice parameters, formation enthalpy ( $\Delta H$ ), and band gaps ( $E_g$ ) of  $\text{Al}_2\text{O}_3$  and  $\text{Ga}_2\text{O}_3$  in corundum ( $\alpha$ - $\text{Al}_2\text{O}_3$  and  $\alpha$ - $\text{Ga}_2\text{O}_3$ ) and monoclinic ( $\theta$ - $\text{Al}_2\text{O}_3$  and  $\beta$ - $\text{Ga}_2\text{O}_3$ ) structures. The indirect and direct band gaps are denoted as (i) and (d), respectively. Note that monoclinic  $\text{Al}_2\text{O}_3$  is often denoted as the  $\theta$  phase in the literature, i.e.,  $\theta$ - $\text{Al}_2\text{O}_3$  shares the same crystal structure as  $\beta$ - $\text{Ga}_2\text{O}_3$  [21–23].

	$\alpha$ - $\text{Al}_2\text{O}_3$		$\theta$ - $\text{Al}_2\text{O}_3$		$\alpha$ - $\text{Ga}_2\text{O}_3$		$\beta$ - $\text{Ga}_2\text{O}_3$	
	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.
$a$ (Å)	4.774	4.76 <sup>a</sup>	11.808	11.795 <sup>b</sup>	5.005	4.983 <sup>c</sup>	12.276	12.214 <sup>d</sup>
$b$ (Å)			2.921	2.910 <sup>b</sup>			3.050	3.037 <sup>d</sup>
$c$ (Å)	13.013	12.99 <sup>a</sup>	5.636	5.621 <sup>b</sup>	13.454	13.433 <sup>c</sup>	5.811	5.798 <sup>d</sup>
$\beta$ (deg)			104.08	103.79 <sup>b</sup>			103.72	103.83
$\Delta H$ (eV/f.u.)	-15.753	-16.971 <sup>e</sup>	-15.561		-9.824		-9.870	-11.30 <sup>f</sup>
$E_g$ (eV)	8.56 (d)	8.8 <sup>g</sup>	7.03 (i)		5.26 (i)	5.3 <sup>h</sup>	4.69 (i)	4.48 <sup>i</sup> , 4.9 <sup>j</sup>

<sup>a</sup>Ref. [24].

<sup>b</sup>Ref. [23].

<sup>c</sup>Ref. [25].

<sup>d</sup>Ref. [26].

<sup>e</sup>Ref. [27].

<sup>f</sup>Ref. [28].

<sup>g</sup>Ref. [29].

<sup>h</sup>Ref. [30].

<sup>i</sup>Ref. [31].

<sup>j</sup>Ref. [32].

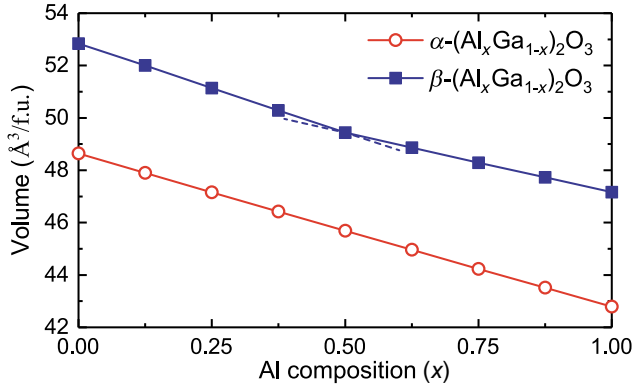


FIG. 2. Calculated equilibrium volume of  $\alpha$  and  $\beta$ -(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> alloys as a function of Al concentration ( $x$ ).

exhibits a change in slope at  $x = 0.5$ . This discontinuity in the slope is attributed to Al occupying the tetrahedral sites for  $x > 0.5$ . This trend was recently observed by Krueger et al. [16].

The calculated formation enthalpies of Ga<sub>2</sub>O<sub>3</sub> and Al<sub>2</sub>O<sub>3</sub>, defined as the total energy of the compound minus the total energies of the elemental bulk phases, are listed in Table I. We find that the formation enthalpy of  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> is only 46 meV/f.u. higher than  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. In contrast,  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> is much more stable than  $\theta$ -Al<sub>2</sub>O<sub>3</sub>, by 192 meV/f.u. This is again attributed to the preference of Al occupying octahedral sites, by  $\sim 0.2$  eV per cation. Figures 3(a) and 3(b) show the formation enthalpies of  $\alpha$  and  $\beta$ -(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub>, defined as

$$\Delta H[(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3] = E[(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3] - xE[\text{Al}_2\text{O}_3] - (1-x)E[\text{Ga}_2\text{O}_3], \quad (1)$$

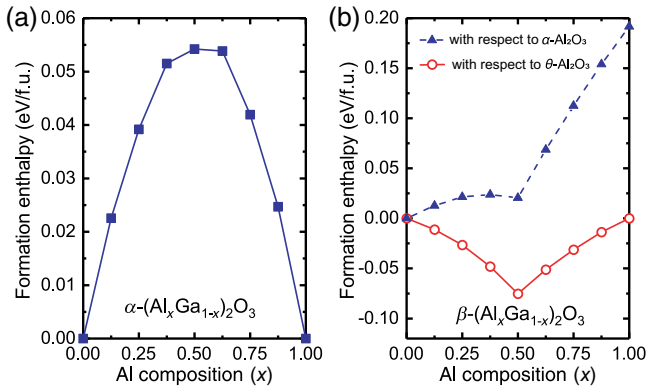


FIG. 3. Formation enthalpies of (a)  $\alpha$  and (b)  $\beta$ -(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> with respect to the parent compounds Ga<sub>2</sub>O<sub>3</sub> and Al<sub>2</sub>O<sub>3</sub>. For  $\beta$ -(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub>, formation enthalpies calculated with respect to  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> +  $\theta$ -Al<sub>2</sub>O<sub>3</sub> (red circles) and  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> +  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> (blue triangles) are shown.

where  $E[(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3]$  is the total energy of the SQS supercell structure representing the random alloy, and  $E[\text{Ga}_2\text{O}_3]$  and  $E[\text{Al}_2\text{O}_3]$  are the total energies of the parent compounds Ga<sub>2</sub>O<sub>3</sub> and Al<sub>2</sub>O<sub>3</sub> in the same supercell. The formation enthalpies of  $\alpha$ -(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> are relatively small compared to other alloys. For example, at  $x = 0.5$ , the formation enthalpy of  $\alpha$ -(In<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> is approximately 300 meV/f.u. [45], compared to 55 meV/f.u. for (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub>. This indicates that  $\alpha$ -(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> alloys are more likely to form at all Al compositions. In the case of  $\beta$ -(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub>, we find a stable ordered compound AlGaO<sub>3</sub> for 50% Al content. If taken with respect to  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> (dashed line), which is the most stable phase of Al<sub>2</sub>O<sub>3</sub>, the formation enthalpy of  $\beta$ -(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> rapidly increases with Al composition above 50%. Again, this is explained by the fact that Al strongly prefer to occupy the octahedral sites for  $x \leq 0.5$ , but end up occupying the only available tetrahedral sites for  $x > 0.5$ .

Therefore, for Al concentrations approaching 100%, we predict that (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> alloys strongly favor the corundum or  $\alpha$  phase. This explains why the single monoclinic phase at  $0 \leq x < 0.8$  and mixed corundum and monoclinic phases for  $0.8 \leq x < 1$  have been observed by solution combustion synthesis [16]. We note, however, that thin films of  $\beta$ -(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> alloys with Al content up to 96% have been reported using PLD [17].

The calculated band gap of (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> alloys as a function of Al content is shown in Fig. 4. The band-gap bowing parameter  $b$  is derived by fitting the results using

$$E_g[(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3] = (1-x)E_g[\text{Ga}_2\text{O}_3] + xE_g[\text{Al}_2\text{O}_3] - bx(1-x). \quad (2)$$

We obtain a bowing parameter of 1.6 eV for  $\alpha$  and 1.0 eV for the  $\beta$ -(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> alloys. Overall, our results are in good agreement with the available experimental data [16–20], also shown in Fig. 4. Due to the stability of the ordered AlGaO<sub>3</sub> ( $x = 0.5$ ), we can define two independent bowing parameters, one for  $0 \leq x \leq 0.5$  and another for  $0.5 \leq x \leq 1$ . These are listed in the Supplemental Material along the bowing parameters for the VBM and conduction-band minimum (CBM) separately [46].

The band offsets between (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> and the parent compound Ga<sub>2</sub>O<sub>3</sub> are crucial parameters in the design of electronic devices that depend on carrier confinement or on the separation between carriers and ionized impurities such as in MODFETs [10,15]. We calculated the band offset between two materials using the following procedure [47]. First, the VBM and the CBM of the bulk materials are determined with respect to the averaged electrostatic potential. Then, we align the averaged electrostatic potential in the two materials by performing an interface calculation. In this case, we used supercells composed of 12 layers of each material with two equivalent interfaces. The supercells are constructed along nonpolar directions to avoid

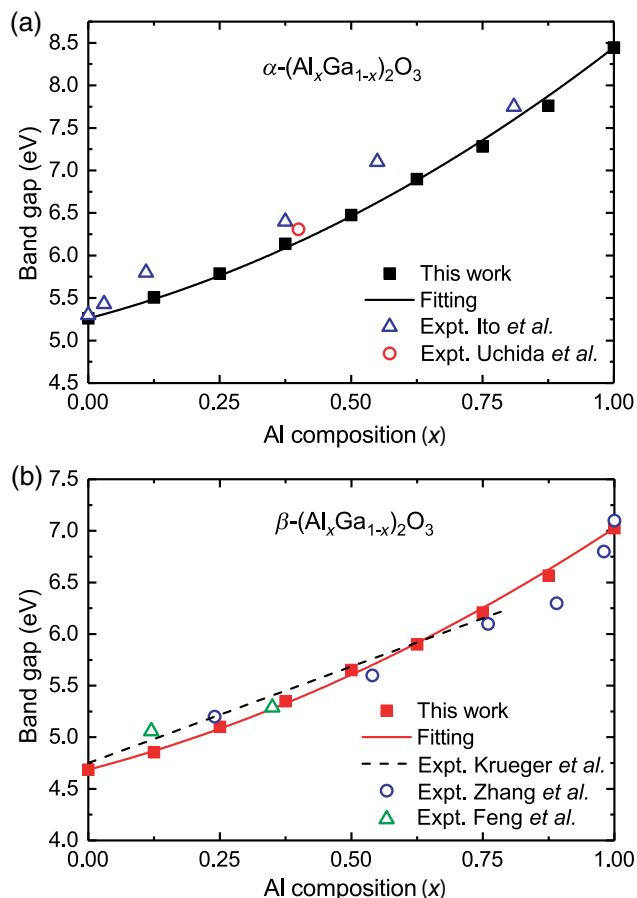


FIG. 4. Band gaps of (a)  $\alpha$  and (b)  $\beta$ -( $\text{Al}_x\text{Ga}_{1-x}$ ) $_2\text{O}_3$  as a function of Al fraction  $x$ . As shown, the calculated results (solid squares) are fitted as solid lines using Eq. (2). The experimental results are from the onset of photoemission inelastic losses in x-ray photoelectron spectroscopy [16], transmittance and x-ray photoelectron spectroscopy [17], energy-loss spectra [19], and optical transmittance and optical absorption spectra [18,20].

problems resulting from the polar discontinuity at the interface and the consequent slopes in the averaged electrostatic potential in the bulk regions. For  $\text{Ga}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3$  in the monoclinic phase, we chose a superlattice geometry along the [010] nonpolar direction. For the corundum phase, we constructed a superlattice along the [100] nonpolar direction. To avoid the problem of lattice mismatch, we used average in-plane lattice parameters; the out-of-plane lattice parameter is set so that each material in the superlattice has its equilibrium volume. In this way, the averaged electrostatic potentials in each side of the interface correspond to the average electrostatic potential in the respective bulk materials. This procedure, therefore, gives us the natural band offset between  $\text{Ga}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3$ .

For monoclinic  $\text{Ga}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3$ , we find a type II staggered alignment, with a valence-band offset of 0.33 eV and a conduction-band offset of 2.67 eV, as shown in Fig. 5(a).

Thus, 89% of the band offset arises from the discontinuity in the conduction band, and only 11% comes from the valence band. In the case of corundum  $\text{Ga}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3$ , we find a type I straddling alignment, with 0.11 eV valence-band offset and 3.19 eV conduction-band offset, also shown in Fig. 5(a), i.e., 97% of the offset comes from the conduction band, and only 3% from the valence band.

We also determined the absolute position of the valence and conduction bands by taking the averaged electrostatic potential of  $\alpha$  and  $\beta$ - $\text{Ga}_2\text{O}_3$  with respect to the vacuum level using surface calculations of nonpolar terminations. The results are shown in the energy axis of Fig. 5(a), where we also added the band-edge positions of amorphous  $\text{Al}_2\text{O}_3$  according to previous experimental results of band gap and valence-band offset with  $\alpha$ - $\text{Al}_2\text{O}_3$  from Ref. [48] for comparison.

Finally, we determined the band-edge positions in ( $\text{Al}_x\text{Ga}_{1-x}$ ) $_2\text{O}_3$  with respect to that in  $\text{Ga}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3$ . The averaged electrostatic potential for a given alloy composition is derived from a linear interpolation of the averaged electrostatic potential of the constituent compounds. Figures 5(b) and 5(c) show the derived VBM and CBM positions for  $\alpha$  and  $\beta$ -( $\text{Al}_x\text{Ga}_{1-x}$ ) $_2\text{O}_3$  as a function of Al composition. The valence-band edges only change slightly with Al concentration  $x$ , while most of the change occurs in the CBM. This is expected since O  $2p$  states dominate the VBM. All the band gap values, the absolute position of VBM and CBM, and the corresponding bowing parameters are listed in the Supplemental Material [46].

The results above have important implications to device design. For instance, for Al concentration of 20% we find that the conduction-band offset between monoclinic ( $\text{Al}_{0.2}\text{Ga}_{0.8}$ ) $_2\text{O}_3$  and  $\text{Ga}_2\text{O}_3$  of 0.47 eV, compared to the assumed 0.6 eV in Ref. [10] for a MODFET structure. This relatively small conduction-band offset for 20% Al content in the alloy can be insufficient so that electrons from the 2DEG at the ( $\text{Al}_{0.2}\text{Ga}_{0.8}$ ) $_2\text{O}_3/\text{Ga}_2\text{O}_3$  may stay in the Si  $\delta$ -doped layer in the ( $\text{Al}_{0.2}\text{Ga}_{0.8}$ ) $_2\text{O}_3$  alloy, causing a parasitic parallel channel of conduction in the MODFET [10]. Higher Al concentrations in the ( $\text{Al}_x\text{Ga}_{1-x}$ ) $_2\text{O}_3$  film ( $\text{Al}_x\text{Ga}_{1-x}$ ) $_2\text{O}_3$ , resulting in increased conduction-band offsets, are required to overcome this detrimental effect.

We also note the discontinuity in the first-order derivative for the CBM and VBM at  $x = 0.5$  for  $\beta$ -( $\text{Al}_x\text{Ga}_{1-x}$ ) $_2\text{O}_3$ . Like the discontinuities in volume and formation enthalpies, this is attributed to Al also occupying tetrahedral sites for  $x > 0.5$ . The kinks at  $x = 0.5$  in the equilibrium volume, formation enthalpies, and band-edge positions of ( $\text{Al}_x\text{Ga}_{1-x}$ ) $_2\text{O}_3$  indicate that  $\beta$ - $\text{AlGaO}_3$  may well be considered an ordered compound with Al in octahedral sites and Ga in tetrahedral sites instead of a random alloy.

In summary, we find that ( $\text{Al}_x\text{Ga}_{1-x}$ ) $_2\text{O}_3$  alloys have much lower mixing enthalpies than ( $\text{In}_x\text{Ga}_{1-x}$ ) $_2\text{O}_3$ . The



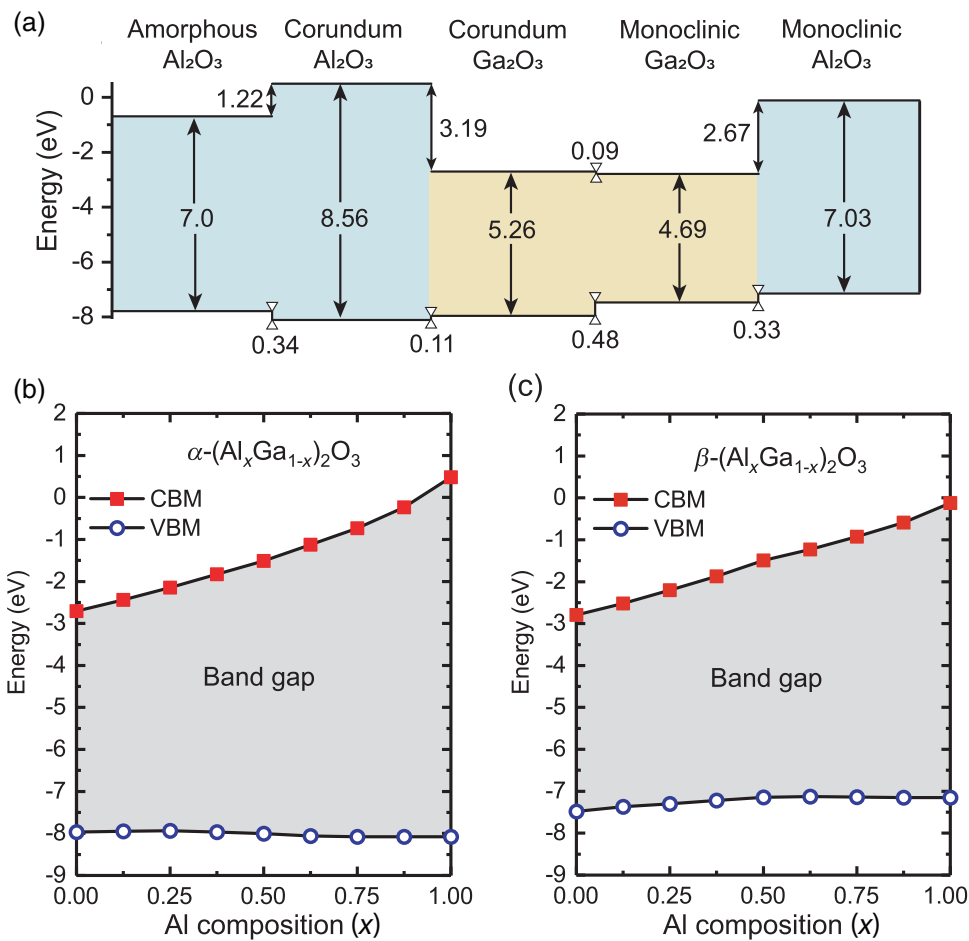


FIG. 5. (a) Calculated band offsets between Ga<sub>2</sub>O<sub>3</sub> and Al<sub>2</sub>O<sub>3</sub>. CBM and VBM positions of (c) α and (d) β-(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub>. The zero in the energy axes corresponds to the vacuum level, determined as described in the text.

band gap of the alloys can be tuned in a wide range by changing Al composition, adding great flexibility in the design of (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub>-based electronic devices. The conduction-band discontinuity comprises 89% of the band offset between monoclinic Al<sub>2</sub>O<sub>3</sub> and Ga<sub>2</sub>O<sub>3</sub>, and 97% in the case of the corundum phase. Our results suggest that films with Al concentrations larger than 20% are required to avoid unwanted parallel conduction channel in MODFETs based on monoclinic (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub> heterostructures.

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