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14. ABSTRACT Binary oxides can sustain extremely high doping levels and exhibit high mobilities. Ga2O3, with a band gap of 4.84 eV, is a highly promising but still relatively unexplored member of this family. The material can be produced in single-crystal form and also be grown epitaxially with high quality. Ga2O3-based metal-semiconductor field-effect transistors have been reported. The material also lends itself to the production of free-standing nanolayers with thicknesses of one or a few monolayers, highlighting its promise as a 2D conductor. During this project we have performed systematic first-principles studies of the following topics: (1) properties of the bulk material, such
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Report Title

Final Report: First-Principles Investigations of Ga₂O₃ and Related Materials as Novel 2D Conductors

ABSTRACT

Binary oxides can sustain extremely high doping levels and exhibit high mobilities. Ga₂O₃, with a band gap of 4.84 eV, is a highly promising but still relatively unexplored member of this family. The material can be produced in single-crystal form and also be grown epitaxially with high quality. Ga₂O₃-based metal-semiconductor field-effect transistors have been reported. The material also lends itself to the production of free-standing nanolayers with thicknesses of one or a few monolayers, highlighting its promise as a 2D conductor. During this project we have performed systematic first-principles studies of the following topics: (1) properties of the bulk material, such as an accurate electronic band structure, phonon spectra, and the effects of strain, characterized by deformation potentials and elastic constants; (2) alloys with In₂O₃ and Al₂O₃; (3) effects of doping, in particular the role of carbon, as well as n-type doping with transition-metals; (4) limitations of the transparency of Ga₂O₃ because of indirect free-carrier absorption; (5) the processes limiting the mobility of free carriers in Ga₂O₃; and (6) the properties of free-standing and embedded nanolayers. The project has resulted in 8 publications, with several more still in progress, and 10 conference talks (including one keynote and 7 invited talks).

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
11/23/2016	2 Daniel Steiauf, John Lyons, Anderson Janotti, Chris Van de Walle. First-principles study of vacancy-assisted impurity diffusion in ZnO, APL Materials, (05 2014): 096101. doi:
11/23/2016	10 H. Peelaers, E. Kioupakis, C. G. Van de Walle. Free-carrier absorption in transparent conducting oxides: Phonon and impurity scattering in SnO ₂ , Physical Review B, (): 235201. doi:
11/23/2016	11 H. Peelaers, C. G. Van de Walle. Doping of Ga ₂ O ₃ with transition metals, Physical Review B, (): 195203. doi:
11/23/2016	12 H. Peelaers, C. G. Van de Walle. Doping of Ga ₂ O ₃ with transition metals, Physical Review B, (): 195203. doi:
TOTAL:	4

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
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TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Chris G. Van de Walle, "First-principles modeling of oxides: bulk properties and inter-faces", E-MRS Fall Meeting, Warsaw, Poland, September 19-22, 2016 (Keynote)

Hartwin Peelaers, "Limits of transparency of transparent conducting oxides" American Physical Society March meeting, Baltimore, MD, March 14-18, 2016 (Invited)

Number of Presentations: 2.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

<u>Received</u>	<u>Paper</u>
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TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

<u>Received</u>	<u>Paper</u>
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TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

08/30/2014 3.00 John L. Lyons, Daniel Steiauf, Anderson Janotti, Chris G. Van de Walle. Carbon as a shallow donor in transparent conducting oxides, PHYSICAL REVIEW A PPLIED (submitted) (08 2014)

08/30/2014 4.00 Hartwin Peelaers, Chris G. Van de Walle. Brillouin zone and band structure of beta-Ga2O3, Physica Status Solidi Rapid Research Letters (08 2014)

TOTAL: 2

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Chris G. Van de Walle was elected to the National Academy for Engineering (NAE) for his "contributions to the theory of semiconductor interfaces and its impact on optoelectronic devices." From the NAE website: "Election to the National Academy of Engineering is among the highest professional distinctions accorded to an engineer. Academy membership honors those who have made outstanding contributions to "engineering research, practice, or education, including, where appropriate, significant contributions to the engineering literature" and to "the pioneering of new and developing fields of technology, making major advancements in traditional fields of engineering, or developing/implementing innovative approaches to engineering education."

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Hartwin Peelaers	0.48
FTE Equivalent:	0.48
Total Number:	1

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Chris G. Van de Walle	0.08	Yes
FTE Equivalent:	0.08	
Total Number:	1	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

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Names of Personnel receiving masters degrees

<u>NAME</u>
Total Number:

Names of personnel receiving PHDs

<u>NAME</u>
Total Number:

Names of other research staff

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
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Report Period Begin Date: 08/01/2015

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Author: Chris G. Van de Walle

Subject Terms (*list keywords that describe the report*): two-dimensional conductors, binary oxides, electronic structure doping, first-principles calculations

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Statement of the problem studied

Binary oxides can sustain extremely high doping levels and exhibit high mobilities. Ga_2O_3 , with a band gap of 4.84 eV, is a highly promising but still relatively unexplored member of this family. The material can be produced in single-crystal form and also be grown epitaxially with high quality. Ga_2O_3 -based metal-semiconductor field-effect transistors have been reported. The material also lends itself to the production of free-standing nanolayers with thicknesses of one or a few monolayers, highlighting its promise as a 2D conductor. During this project we have performed systematic first-principles studies of the following topics: (1) properties of the bulk material, such as an accurate electronic band structure, phonon spectra, and the effects of strain, characterized by deformation potentials and elastic constants; (2) alloys with In_2O_3 and Al_2O_3 ; (3) effects of doping, in particular the role of carbon, as well as n -type doping with transition-metals; (4) limitations of the transparency of Ga_2O_3 because of indirect free-carrier absorption; (5) the processes limiting the mobility of free carriers in Ga_2O_3 ; and (6) the properties of free-standing and embedded nanolayers. The project has resulted in 8 publications, with several more still in progress, and 10 conference talks (including one keynote and 7 invited talks).

Summary of the most important results

1. Ga_2O_3 : bulk properties

The stable phase of Ga_2O_3 is the monoclinic beta phase. Given the low symmetry of this phase, the Brillouin zone is expected to be complicated (**Figure 1**). In fact, prior to our study [P5], all published band structures of Ga_2O_3 were based on an incorrect Brillouin zone. Often, the reciprocal unit cell was used instead of the correct zone. We have addressed these issues, while at the same time providing a very accurate description of the electronic properties, including values for the effective masses, the correct position of the indirect band gap, and the location of secondary conduction-band minima.

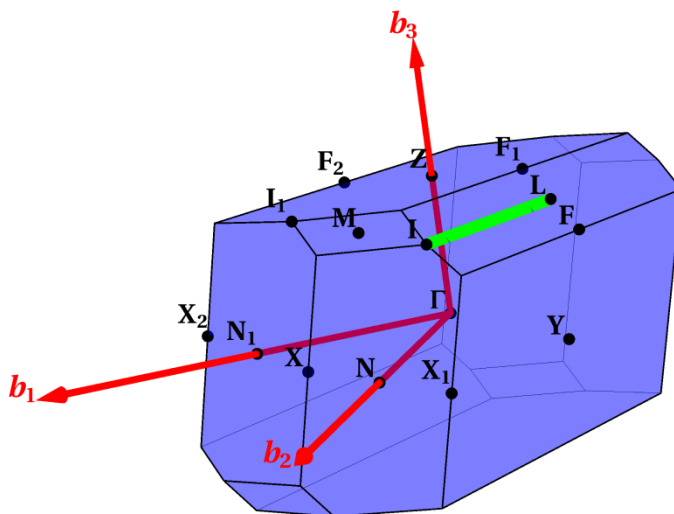


Figure 1: Calculated Brillouin zone of monoclinic Ga_2O_3 . High-symmetry points are indicated.

We have also calculated the phonon spectrum of Ga₂O₃, shown in **Figure 2**. The discontinuities at the Γ point are caused by the low symmetry of the crystal: the response to the electric field induced by the longitudinal optical phonon modes depends strongly on the crystal direction. We have used this phonon spectrum as the basis for our calculations of the indirect absorption spectra (see Sec. 4) and the mobility (see Sec. 5).

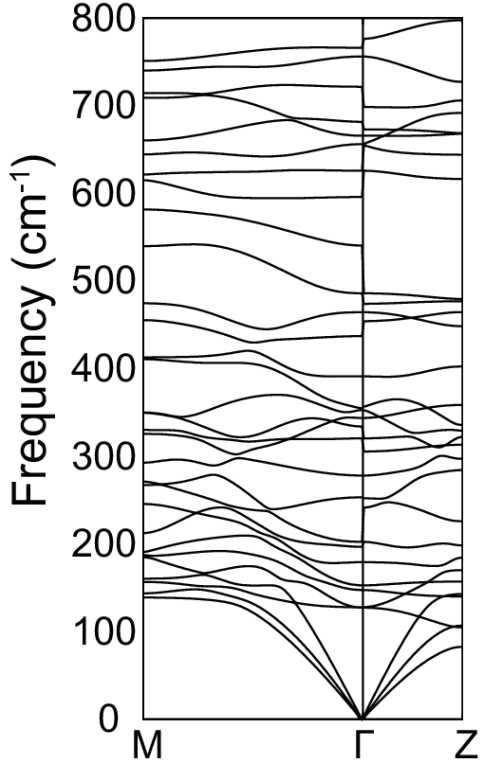


Figure 2: Phonon band structure of Ga₂O₃ along two high-symmetry directions. The discontinuities at Γ are due to the low symmetry of the crystal.

When Ga₂O₃ is grown epitaxially on a substrate with different lattice parameters, or when it is subject to an externally applied stress, it will be strained. This will lead to a change in the electronic properties. Knowledge of the effect of strain on the electronic structures is important for device applications. To characterize this effect we calculated the deformation potentials, which give the proportionality factors between the change in band gap and the strain in a certain direction. **Table 1** lists the deformation potentials along the Cartesian directions. For the normal components (*xx*, *yy*, and *zz*), the sign of the deformation potential is negative, indicating that tensile strain will reduce the band gap. The shear components have smaller deformation potentials than the normal components.

	Deformation potential for the direct band gap (eV)	Deformation potential for the indirect band gap (eV)
D_{xx}	-8.04	-7.60
D_{yy}	-10.68	-8.28
D_{zz}	-6.74	-8.70
D_{xy}	-0.15	-0.17
D_{xz}	-1.48	0.30
D_{yz}	0.01	-0.02

Table 1: Deformation potentials along the Cartesian directions for bulk Ga₂O₃.

A related quantity are the elastic constants, which describe the proportionality between stress and strain. Given the low symmetry of the monoclinic lattice, Ga_2O_3 has 13 different elastic constants. Our calculated values, listed in **Table 2**, are being used by our experimental collaborators in the Speck group at UCSB to characterize $\text{Al}_2\text{O}_3/\text{Ga}_2\text{O}_3$ alloy compositions (see next section for our theoretical study of these alloys) by measuring the peak splitting in x-ray diffraction spectra.

	xx	yy	zz	yz	xz	xy
xx	259	135	151	0	-25	0
yy	135	386	102	0	8	0
zz	151	102	377	0	7	0
yz	0	0	0	64	0	21
xz	-25	8	7	0	80	0
xy	0	0	0	21	0	100

Table 2: Calculated elastic constants of Ga_2O_3 .

2. Alloys of In_2O_3 or Al_2O_3 and Ga_2O_3

As mentioned before, the most stable phase of Ga_2O_3 is the monoclinic phase, while the most stable phase of In_2O_3 is the cubic bixbyite structure. We have calculated band alignments between the materials in each of these phases [P6]. When an alloy of both materials is formed, it is not a priori known what crystal structure will be formed. Such alloys allow engineering lattice parameters and band gaps.

We find (**Figure 3**) that in both the monoclinic and bixbyite structures, the lattice parameters vary linearly with concentration (Vegard's law). The band gap also varies approximately linearly for the monoclinic structure, but exhibits a large band-gap bowing in the bixbyite structure. We also found that the difference between the dipole-forbidden fundamental gap and the dipole-allowed gap is larger for alloys containing more In.

The monoclinic structure can incorporate In favorably for concentrations less than 50%. Higher concentrations preferably form in the bixbyite structure. This can be explained by considering the differences in coordination of the Ga/In atoms in monoclinic versus bixbyite: in the monoclinic structure, half the Ga/In sites are tetrahedrally coordinated, and the remainder are octahedrally coordinated; in contrast, in bixbyite all sites are octahedrally coordinated. Indium atoms strongly prefer octahedral coordination, explaining why only concentrations up to 50% are favorable in the monoclinic structure. Our publication detailing these results [P6] was selected as an Editor's Suggestion.

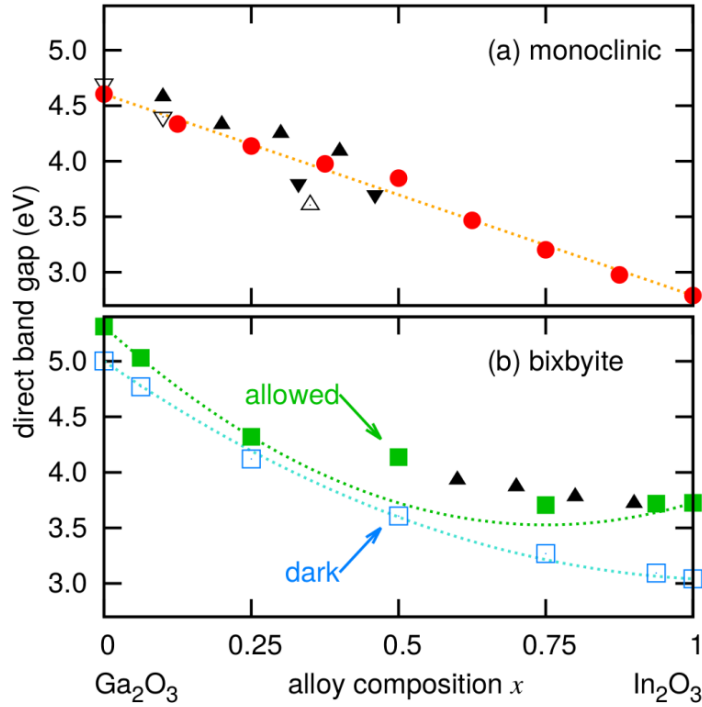


Figure 3: Direct band gap at Γ for ordered $(\text{In}_x\text{Ga}_{1-x})_2\text{O}_3$ alloys. (a) For the monoclinic Ga_2O_3 structure (red circles), the orange line is a linear interpolation between the binary compounds. (b) In the bixbyite structure, the blue open squares denote the band gap corresponding to the average of the three highest valence bands; this gap is dark. The lines are parabolic fits. The green solid squares denote the lowest direct transition at Γ with a large dipole matrix element. Other symbols denote experimental values from the literature. From Ref. [P6].

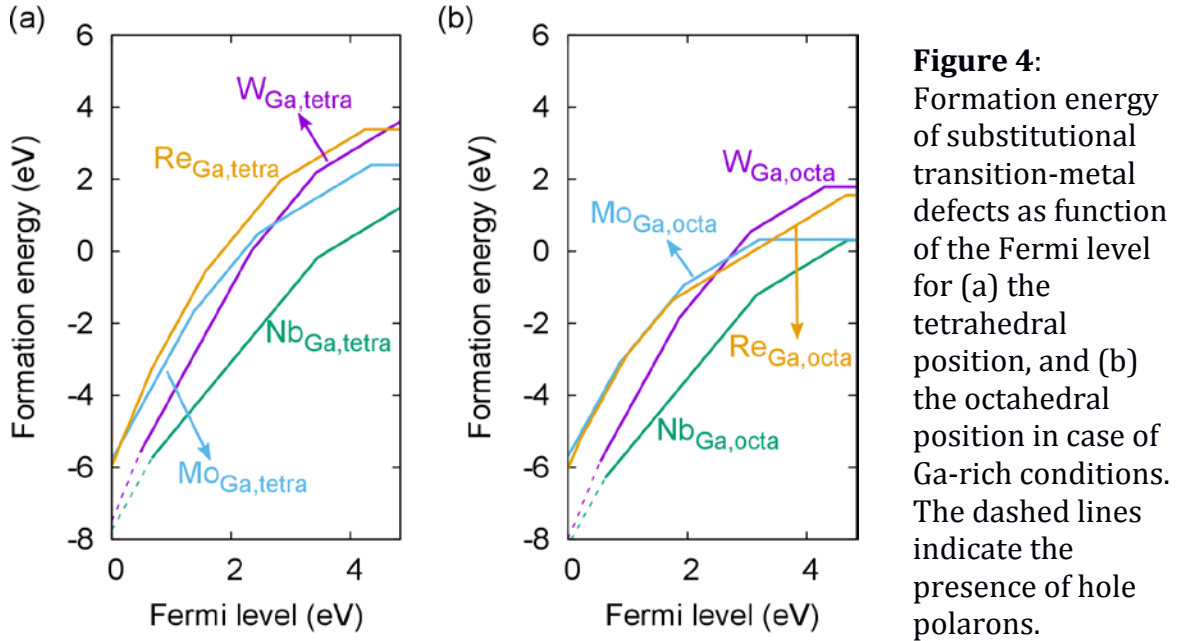
In contrast to In_2O_3 , the most stable phase of Al_2O_3 is the corundum structure. This structure contains only octahedrally coordinated positions. Similar to the $(\text{In}_x\text{Ga}_{1-x})_2\text{O}_3$ alloys, we find a linear change in the lattice parameters of $(\text{In}_x\text{Al}_{1-x})_2\text{O}_3$ alloys with concentration. However, both the corundum and the bixbyite structures show a bowing in the band gaps. The monoclinic structure is the preferred structure for Al concentrations up to 50%. Our experimental colleagues at UCSB are currently growing various alloys using molecular beam epitaxy (MBE). Preliminary results show good agreement with our calculations. A publication is in preparation.

3. Doping

For device applications it is important to achieve high carrier concentrations and high mobility in Ga_2O_3 . In this section we will focus on achieving high doping levels; mobility will be discussed in Section 5.

We examined the effect of carbon doping in Ga_2O_3 [P3, P4]. Carbon is often an unintentional contaminant in the growth process, e.g., in metal-organic chemical vapor deposition (MOCVD). We found that, depending on the growth conditions, C can incorporate on the Ga site and act as a shallow donor, or it can incorporate on an O site, acting as a deep acceptor. The latter situation is preferred in O-poor conditions, which occur when the material is grown using MBE, or when the metal-organic precursors are not completely decomposed in MOCVD. Since carbon on an oxygen site will compensate the n -type conductivity, its presence is highly undesirable. It might be the cause of some of the observed difficulties in achieving high concentrations of free carriers.

Gallium vacancies are also potentially detrimental defects; they act as a triple acceptor [Varley 2011]. The presence of gallium vacancies has been observed by positron annihilation experiments in Sn-doped Ga_2O_3 [Korhonen 2015]. We will comment on the effect of vacancies on mobility in Section 5.



We also considered non-traditional doping routes to achieve n -type conductivity. In particular, we considered doping with the transition metals Mo, W, Nb, and Re. All these transition metals prefer high-spin states when incorporated on the Ga site. The unpaired electrons causing the magnetic moment to have distinct d character. Substitution on the octahedral Ga sites is lower in energy compared to the Ga tetrahedral sites. These transition metals are generally deep donors. The main exception is Nb, which is a shallow donor when it substitutes on a tetrahedral site, and has a small enough ionization energy to enable n -type conductivity on the octahedral site. Niobium also has the lowest formation energy among the considered transition metal impurities. A plot of the formation energies is shown in **Figure 4**. These results have been published in Physical Review B [P8].

When Ga_2O_3 is n -type doped, the Fermi level will increase and the conduction band will start to be filled with electrons. This filling causes two observable effects: the observed optical band gap will increase (Burstein-Moss shift), as direct optical transitions can occur only from an occupied state to an unoccupied state. Due to the filling of the conduction band these unoccupied states will lie higher in energy. At the same time this conduction-band filling will increase the observed electron effective mass, since the curvature of the bands changes with energy. **Figure 5** shows both effects: the shift in Fermi level with doping concentration, and the corresponding increase in electron effective mass. These results are obtained by integration of a very accurate Wannier-interpolated band structure.

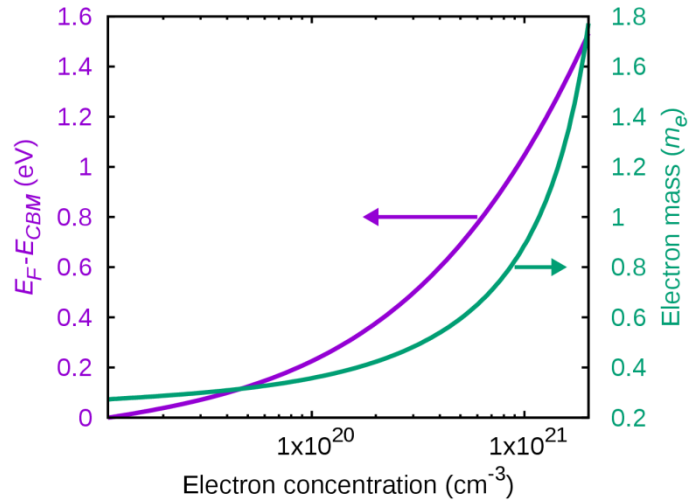


Figure 5: The position of the Fermi level (left axis) and the corresponding electron effective mass (right axis) as a function of the free-carrier concentration.

4. Free-carrier absorption

The large band gap of Ga₂O₃ (4.84 eV indirect and 4.88 eV direct) makes Ga₂O₃ an ideal candidate for a transparent conducting oxide (TCO), where the transparency is extended to the UV region. This enables a wide range of applications, such as transparent contacts in solar cells and other optoelectronic devices. In order to make Ga₂O₃ conducting, free carriers need to be introduced (see Section 3 for a discussion on doping). These free carriers can lead to additional absorption processes: direct absorption to higher conduction-band states, which requires a large photon energy because of the large dispersion of the lowest conduction band, and indirect processes, which can be intraband and therefore require less photon energy, but require an additional scattering process to provide the necessary momentum. Phonons can provide this momentum.

We built on a methodology, based on Fermi's golden rule, which we previously applied to describe free-carrier absorption in SnO₂ [Peelaers 2012]. We extended this methodology [P7] and then performed a detailed study of indirect absorption in Ga₂O₃ [Figure 6]. Similar to indirect absorption in SnO₂ we find that in Ga₂O₃ the indirect *intraband* absorption increases with decreasing photon energy (increasing wavelength). This behavior is typically described with a Drude expression fitted to experiment, but now we are able to describe it completely from first principles.

Given the large band gap of Ga₂O₃, also direct and indirect *interband* transitions are possible, leading to an increase in absorption, for light polarized along the y direction, at energies of around 3.2 and 4.3 eV. Such interband transitions were not possible in SnO₂ (which has a gap of 3.6 eV).

We conclude that for applications that require transparency in the visible light region, Ga₂O₃ is a very good material, but for UV light applications, one should take this increase

in absorption at specific wavelengths into account. Note that the polarization of the light is important, as not all transitions to the higher conduction bands are dipole allowed. We are preparing a manuscript detailing these results.

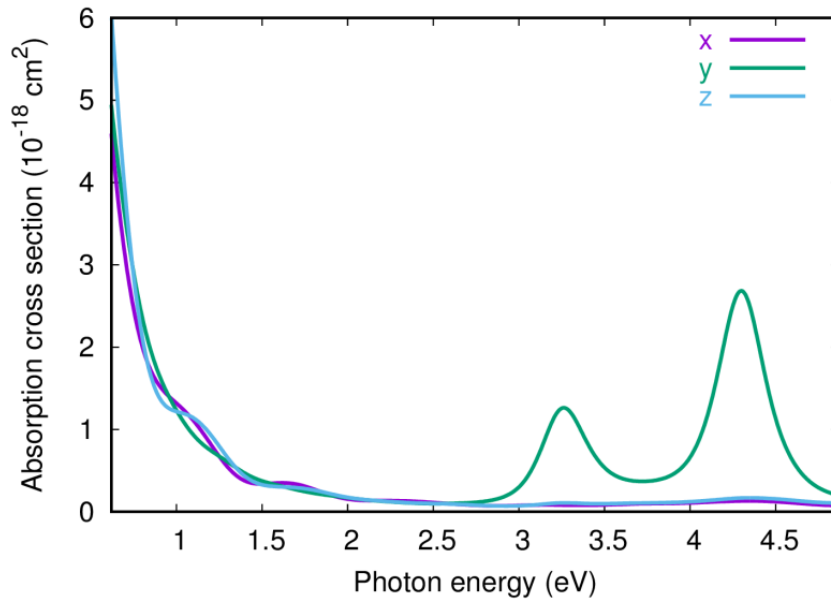


Figure 6: Calculated indirect-absorption cross section due to phonons for light polarized along the three Cartesian directions.

5. Mobility of Ga₂O₃

For device applications it is important to have both a high free-carrier concentration (see Section 3 for different doping strategies) and a high mobility. We have performed a detailed first-principles study of mobility limited by phonon scattering and charged impurity scattering. Our methodology is based on solving the Boltzmann transport equation in the relaxation-time approximation. The scattering times were calculated using Fermi's golden rule. The main phonon scattering process is scattering by longitudinal optical phonons. To describe this we use the Vogl model, which fully takes into account the anisotropy of the phonon modes and also multiple phonon modes (in contrast to the often used Fröhlich model, which is isotropic and only considers a single longitudinal optical phonon mode). The ionized impurity scattering is modeled using a Yukawa potential. The screening due to the free carriers is explicitly taken into account in both processes.

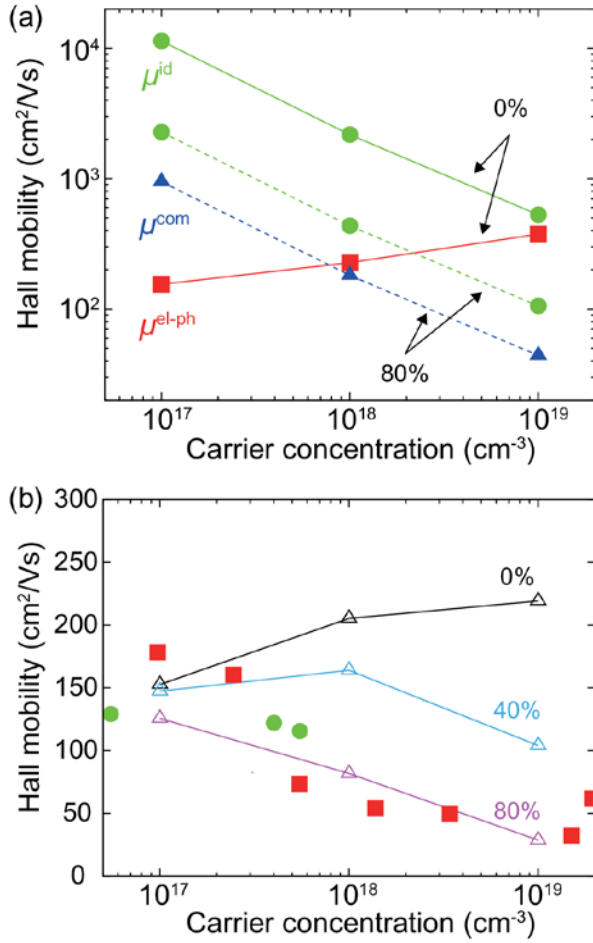


Figure 7: (a) Hall mobility due to three different limiting processes: scattering with phonons (μ^{el-ph}), scattering with ionized donors (μ^{id}), and scattering with compensating defects (μ^{com}). We used two different levels of compensation (0% and 80%). (b) Total mobility due to all processes, for different amounts of compensation, compared to experimental measurements (full squares and circles).

In contrast to what some experimental results suggested [Ueda 1997], we find that the scattering times are only slightly anisotropic, which is surprising given the high anisotropy of the phonon modes. We also find that for small carrier concentrations, the mobilities are mainly limited by scattering due to longitudinal optical phonons [see **Figure 7(a)**]. The scattering due to ionized donors only becomes comparable in importance when the free-carrier concentrations are larger than 10^{19} cm⁻³. When comparing to experimental results [Irmischer 2011, Sasaki 2012], as shown in **Figure 7(b)**, we obtain very good agreement for the low carrier concentrations, but predict too high a mobility for larger carrier concentrations compared to the experimental results of. This discrepancy can be resolved if we take into account the presence of compensating Ga vacancies, which have been observed experimentally [Korhonen 2015]. If we assume 80% donor compensation, our results agree well with experimental observations for all considered carrier concentrations. A paper detailing our methodology and these results is in preparation.

6. Layered Ga₂O₃

In work that was partially funded by the grant, our experimental collaborators found that it is possible to mechanically cleave bulk Ga₂O₃ and create thin Ga₂O₃ nanomembranes [P1]. These nanolayers prefer to be terminated by (100)B surfaces, and the minimum width is half the conventional unit cell. We define this width as w (with a value of 5.94 Å) (see **Figure 8**). In most materials, lowering the dimensionality usually leads to major changes in electronic properties. The most noticeable change is expected to be due to quantum confinement, which increases the band gap.

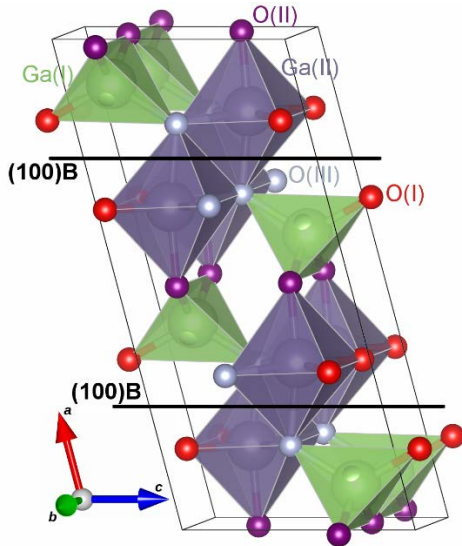


Figure 8. Unit cell of monoclinic Ga_2O_3 , with polyhedra indicating the tetrahedral (green) and octahedral (purple) sites. The volume between the horizontal lines denotes the smallest possible Ga_2O_3 layer, with width w .

Remarkably, our calculations show that no such effect is observed in thin Ga_2O_3 nanolayers: the band gap (both direct and indirect) remains similar to the bulk band gap, and also the electron effective masses are unchanged. This can be observed in the band structures shown in **Figure 9**. We are able to explain this seeming lack of quantum confinement by the presence of a gallium dangling bond state on the surface of the nanolayer.

Our study of Ga_2O_3 layers embedded in Al_2O_3 , which has a larger band gap, can also shed more light on this. Now there is no Ga dangling bond, since bonds are formed between the Ga_2O_3 and Al_2O_3 . In this case, the effects of quantum confinement can indeed be observed. Our calculated band structures [**Figure 10(a)-(b)**] show that the lowest conduction bands are due to the Ga_2O_3 nanolayer, and that both the band gap and the electron effective masses are increased compared

to the bulk values. The isosurface of the charge density corresponding to the conduction-band minimum (at Γ) [**Figure 10(c)**] shows that there is no gallium dangling bond state.

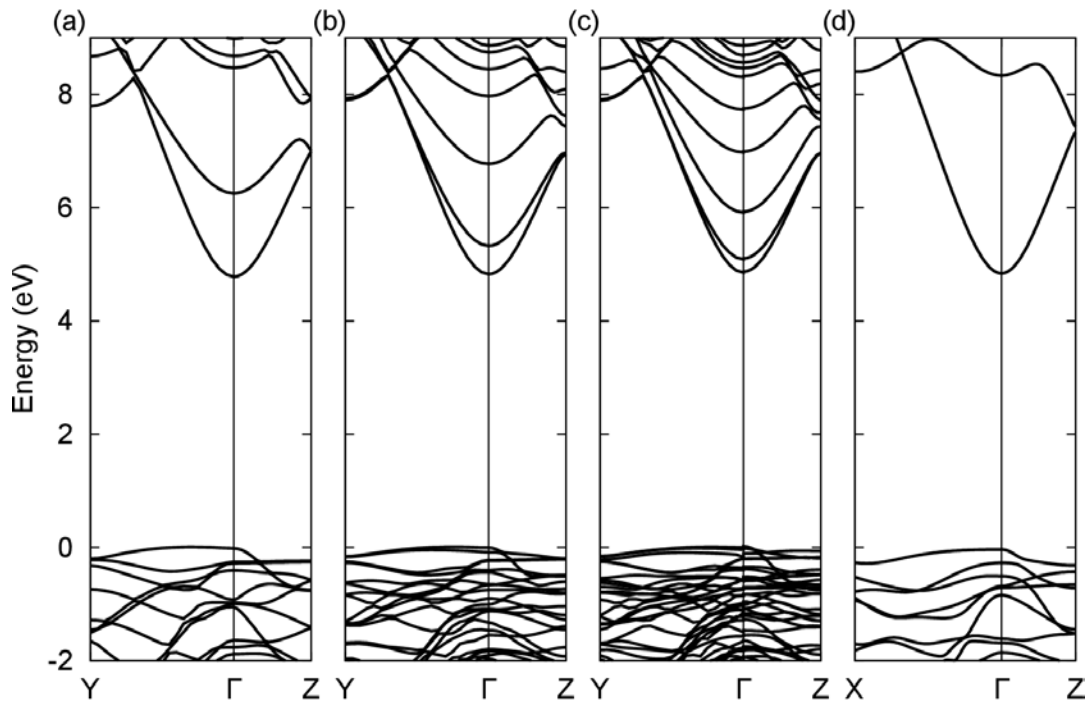


Figure 9: Calculated band structures for Ga_2O_3 nanolayers. The width of the nanolayer is increased from $1w$ (5.94 \AA) in (a) to $2w$ in (b) and $3w$ in (c). (d) shows the corresponding band structure of bulk Ga_2O_3 .

These observations are consistent with our explanation that this dangling-bond state obscures the quantum-confinement effect in free-standing nanolayers. Embedding within a larger band-gap material does lead to quantum confinement and larger band gaps. A paper discussing free-standing and embedded nanolayers is in preparation.

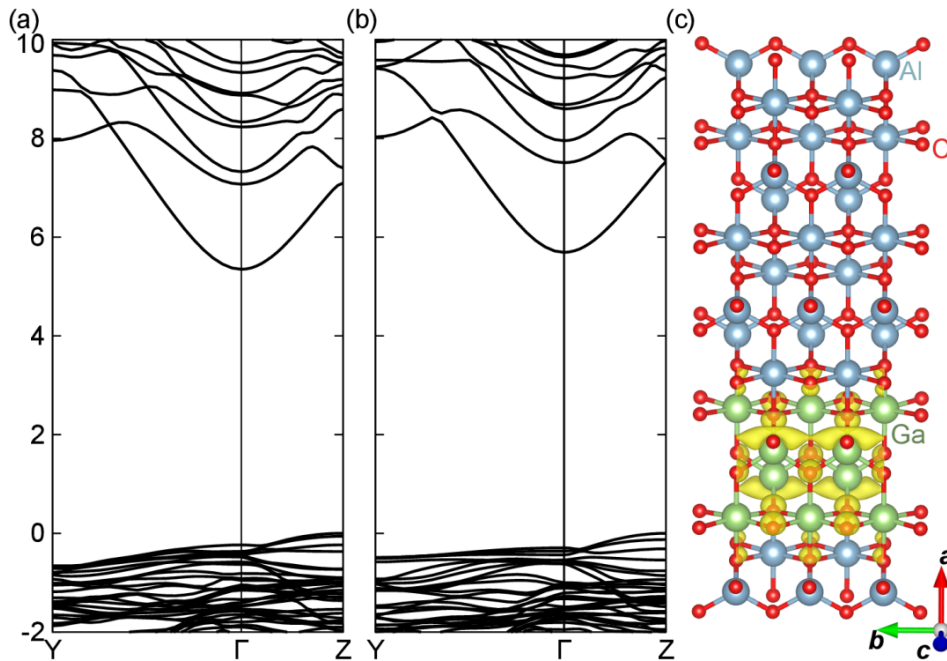


Figure 10: Band structure of a nanolayer of Ga₂O₃ [with width w (5.94 Å)] embedded in monoclinic Al₂O₃, with (a) lattice parameters constrained to the in-plane Ga₂O₃ lattice parameters, and (b) to the Al₂O₃ lattice parameters. (c) Isosurface indicating 10% of the maximum charge density corresponding to the lowest conduction band at Γ for the band structure shown in (a).

In previous work [Varley 2012] we showed that in bulk Ga₂O₃ holes form self-trapped polarons. These polarons can localize on the three different symmetry-inequivalent oxygen atoms. For two of the O sites [O(I) and O(II); see **Figure 8**] the polaron is more stable than the delocalized hole, and only small relaxations of the lattice occur. A polaron on the O(III) site, however, is not stable compared to a delocalized hole; this polaron also leads to a large lattice distortion. Our experimental colleagues from the Leibniz Institute for Crystal Growth, Berlin, used time-dependent transmission electron microscopy to study Ga₂O₃ layers. They observed atomic motion consistent with the displacement patterns of the polaron on the O(III) site. This raised the question if it is possible to localize polarons in Ga₂O₃ nanolayers, and if so, if they exhibit similar displacement patterns. To address this question, we developed a methodology to simulate charged slabs. Such a new methodology was required, since the standard approach to treat charged systems in periodic boundary conditions leads to divergences in lower dimensions. Our calculations confirmed that it is possible to localize polarons in thin nanolayers, and that the displacement pattern of a polaron localized on a O(III) atom matches the experimental observation. A paper detailing both experimental and computational findings is in preparation.

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Appendix: Publications, Presentations, Honors and Awards

Publications

- [P1] “**High-voltage field effect transistors with wide-bandgap β -Ga₂O₃ nanomembranes**”, W. S. Hwang, A. Verma, H. Peelaers, V. Protasenko, S. Rouvimov, H. G. Xing, A. Seabaugh, W. Haensch, C. Van De Walle, Z. Galazka, M. Albrecht, R. Fornari, and D. Jena, Appl. Phys. Lett. **104**, 203111 (2014). [doi:10.1063/1.4879800]
- [P2] “**First-principles study of vacancy-assisted impurity diffusion in ZnO**”, D. Steiauf, J. L. Lyons, A. Janotti, and C. G. Van de Walle, APL Materials **2**, 096101 (2014). [doi: 10.1063/1.4894195]
- [P3] “**Carbon as a shallow donor in transparent conducting oxides**”, J. L. Lyons, D. Steiauf, A. Janotti, and C. G. Van de Walle, Phys. Rev. Appl. **2**, 064005 (2014). [doi: 10.1103/PhysRevApplied.2.064005]
- [P4] “**Carbon-induced trapping levels in oxide dielectrics**”, H.D. Taylor, J. L. Lyons, M. Choi, A. Janotti, and C.G. Van de Walle, J. Vac. Sci. Tech. A **33**, 01A120 (2015). [doi: 10.1116/1.4901234]
- [P5] “**Brillouin zone and band structure of β -Ga₂O₃**”, H. Peelaers and C. G. Van de Walle, Phys. Status Solidi B **252**, 828 (2015). [doi: 10.1002/pssb.201451551]
- [P6] “**(In_xGa_{1-x})₂O₃ alloys for transparent electronics**”, H. Peelaers, D. Steiauf, J. B. Varley, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **92**, 085206 (2015). [doi:10.1103/PhysRevB.92.085206]
- [P7] “**Free-carrier absorption in transparent conducting oxides: Phonon and impurity scattering in SnO₂**”, H. Peelaers, E. Kioupakis, and C.G. Van de Walle, Phys. Rev. B **92**, 235201 (2015). [doi: 10.1103/PhysRevB.92.235201]
- [P8] “**Doping of Ga₂O₃ with transition metals**”, H. Peelaers and C. G. Van de Walle, Phys. Rev. B **94**, 195203 (2016). [doi: 10.1103/PhysRevB.94.195203]

Presentations

- Chris G. Van de Walle, “First-principles modeling of oxides: bulk properties and interfaces”, E-MRS Fall Meeting, Warsaw, Poland, September 19-22, 2016 (**Keynote**)
- Hartwin Peelaers, “Limits of transparency of transparent conducting oxides” American Physical Society March meeting, Baltimore, MD, March 14-18, 2016 (**Invited**)
- Chris G. Van de Walle, “Optoelectronic Materials: Transparent Conductors and Light Emitters”, Workshop on Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany, July 13-23, 2015. (**Invited**)

Chris G. Van de Walle, "Controlling the properties of two-dimensional conductors", Workshop on Advances in Modeling of Nano Materials, Hefei, China, June 14-16, 2015. **(Invited)**

Hartwin Peelaers, "Polarons in thin Ga_2O_3 layers", American Physical Society March meeting, San Antonio, TX, March 2-6, 2015.

Chris G. Van de Walle, "Transparent conductors for energy and electronics", 9th International Conference on Computational Physics (ICCP9), National University of Singapore, Singapore, January 7-11, 2015. **(Invited)**

Hartwin Peelaers, "Polarons in thin Ga_2O_3 layers", ICMR Workshop on Charged Systems and Solid/Liquid Interfaces", Santa Barbara, CA, July 6-11, 2014.

Chris G. Van de Walle, "Effects of high doping in transparent conductors", CECAM Workshop on Nanostructured Zinc Oxide and related materials, Bremen, Germany, June 23-27, 2014. **(Invited)**

Hartwin Peelaers, "Fundamental limits on optical transparency of transparent conducting oxides", 13th International Conference on Modern Materials and Technologies: 6th Forum on New Materials, Montecatini Terme, Italy, June 15-19, 2014. **(Invited)**

Chris G. Van de Walle, "Controlling the conductivity of two-dimensional conductors", Electronic Materials and Applications 2014, American Ceramic Society, Orlando, Florida, January 22-24, 2014. **(Invited)**

Honors and Awards

Chris G. Van de Walle was elected to the National Academy of Engineering (NAE) for his "contributions to the theory of semiconductor interfaces and its impact on optoelectronic devices." From the NAE website: "Election to the National Academy of Engineering is among the highest professional distinctions accorded to an engineer. Academy membership honors those who have made outstanding contributions to "engineering research, practice, or education, including, where appropriate, significant contributions to the engineering literature" and to "the pioneering of new and developing fields of technology, making major advancements in traditional fields of engineering, or developing/implementing innovative approaches to engineering education."

Chris G. Van de Walle received the 2015 TMS John Bardeen Award. The award recognizes his "seminal contributions to the theory and understanding of semiconductor band offsets, doping, defects, and loss mechanisms, and the role of hydrogen in electronic materials".

Chris G. Van de Walle has been included in the 2014 “Highly Cited Researchers” list (www.highlycited.com). The distinction is awarded to researchers who wrote the greatest numbers of reports officially designated by Essential Science IndicatorsSM as Highly Cited Papers—ranking among the top 1% most cited for their subject field and year of publication, earning them the mark of exceptional impact.

Chris G. Van de Walle is the inaugural recipient of the Herbert Kroemer Endowed Chair in Materials Science. His appointment recognizes his outstanding achievements in computational materials science, where he has employed first-principles techniques to model the structure and behavior of wide-band-gap semiconductors, oxides, and hydrogen storage materials.

Chris G. Van de Walle received the 2013 AVS Medard W. Welch Award, the premier honor given by AVS, the Science and Technology society. The citation reads "For seminal contributions to the theory of heterojunctions and its applications to semiconductor technology, and for elucidating the role of hydrogen in electronic materials."