Boron doping in gallium oxide from first principles

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We study the feasibility of boron doping in gallium oxide (Ga$_2$O$_3$) for neutron detection. Ga$_2$O$_3$ is a wide band-gap, radiation hard material which has potential for neutron detection if it can be doped with a neutron active element. We investigate the boron-10 isotope ($^{10}$B) as possible neutron active dopant. Intrinsic and boron induced defects in Ga$_2$O$_3$ are studied with semi-local and hybrid density-functional-theory calculations. We find that in growth conditions favourable for boron, boron substitutional defects are likely to form making boron doping of Ga$_2$O$_3$ feasible.

I. INTRODUCTION

Gallium oxide (Ga$_2$O$_3$) is a wide gap semiconductor (band gap $E_g \sim 4.9$ eV [1]) with potential applications in ultraviolet optoelectronic devices, power electronics and laser lithography [2–7]. In this work, we are exploring further applications of Ga$_2$O$_3$ for neutron detectors. There is a growing need for neutron detectors with low-power requirements, compact size and reasonable resolution for, e.g., non-invasive neutron imaging of organic materials, like human tissue or wood [8], safeguarding and non-proliferation of nuclear material [9], safety in the nuclear industry [10], space science [11] and autonomous radiation probes for hazardous environments [12].

Most current neutron detectors use helium-3 gas ($^3$He), a non-radioactive isotope of helium, because of its extreme sensitivity in detecting neutron radiation [9–13]. However, innovation is greatly needed, since current neutron detectors are expensive, bulky and not radiation hard precisely because of their use of $^3$He. The world’s $^3$He supply is extremely scarce and depleting rapidly. Moreover, the large size of $^3$He detectors limits their portability and spatial resolution. Since $^3$He detectors are not radiation hard they cannot be used in harsh environments like outer space, or fusion or nuclear reactors. For these reasons, semiconductor detectors have recently received increasing attention [14–18]. However, the materials requirements for optimal energy, time and spatial resolution, detection efficiency, robustness and radiation hardness are daunting challenges [13], and there is currently no satisfying material choice nor commercially available semiconductor detectors. For this reason, we are here exploring Ga$_2$O$_3$ as potential neutron detector material.

Solid state neutron detectors use neutron active elements, which convert neutrons to electronic excitation via a nuclear reaction. The ability of neutron active elements to capture neutrons is measured by the neutron cross section. The boron isotope $^{10}$B has the largest neutron cross-section at 3840 barns, which is comparable to helium $^3$He and larger than other candidates like lithium ($^6$Li) and beryllium ($^9$Be). Boron-based neutron detectors have recently been demonstrated experimentally [15–18], but are far from commercialisation. Wide band-gap materials have also been investigated in solid state neutron detectors, most notably gallium nitride (GaN) [19–20]. Here, we consider beta gallium oxide ($\beta$-Ga$_2$O$_3$) as potential material for neutron detection, because $\beta$-Ga$_2$O$_3$ is a radiation hard wide band-gap material, and gallium has similar chemical characteristics as boron which makes boron implantation on gallium sites favorable.

The electronic structure of $\beta$-Ga$_2$O$_3$ and the behavior of defects in the material have attracted considerable interest and have been studied previously with density function theory (DFT) [11,19–20]. Defects have been investigated as a source of the observed intrinsic n-type conductivity and for the possibility of p-type doping of $\beta$-Ga$_2$O$_3$ for opto-electronic applications. Boron-related defects have not been previously studied in $\beta$-Ga$_2$O$_3$.

We here investigate the possibility of boron doping with DFT. With the supercell approach, we calculate formation energies for simple point defects and complexes in $\beta$-Ga$_2$O$_3$ in the diffuse doping limit. We study both intrinsic defects and boron defects to assess the feasibility of introducing boron to $\beta$-Ga$_2$O$_3$. Our work provides insight into the limits of boron doping and the potential of $\beta$-Ga$_2$O$_3$ for neutron detection.

The article is structured as follows. First, we discuss the atomic structure of $\beta$-Ga$_2$O$_3$ and present the computational methods used in this work (Section II). We then investigate the intrinsic defects found in $\beta$-Ga$_2$O$_3$ (Section III-B). Finally, we study boron defects and compare them to the intrinsic defects (Section III-C) before concluding our work (Section IV).

II. COMPUTATIONAL DETAILS

$\beta$-Ga$_2$O$_3$ has a monoclinic crystal structure with space group C2/m. The unit cell contains two nonequivalent gallium sites and three nonequivalent oxygen sites. The monoclinic cell with 4 Ga$_2$O$_3$ units (i.e., 20 atoms) is shown in Fig. 1. The five different sites are labeled Ga(I), Ga(II), O(I), O(II) and O(III). The gallium sites Ga(I) and Ga(II) are tetrahedrally and octahedrally coordinated by O ions, respectively. The O(III) site is four-fold coordinated, while both O(I) and O(II) are three-fold coordinated. An O(I) site has two Ga(II) and one Ga(I) as neighbors, while an O(II) has two Ga(I) and one Ga(II) neighboring sites.

All defect calculations were carried out with the su-
Point defects were introduced in a 160-atom supercell model of pristine β-Ga$_2$O$_3$, i.e., 32 Ga$_2$O$_3$ units. Following Ref. [21] we calculated the defect formation energy according to

$$E_i(X^q) = E(X^q) - E(0) - \sum \Delta n_i \mu_i + q(\epsilon_{\text{VBM}} + \epsilon_F) + E_{\text{corr}},$$

(2.1)

where $E(X^q)$ is the DFT total energy of the supercell containing a defect in charge state $q$, and $E(0)$ the total energy of the defect-free crystal. $\mu_i$ is the chemical potentials of the $i$th species whose number varies by $\Delta n_i$ when defects are formed. $\Delta n_i$ is negative for the removal of atoms (e.g., vacancies) and positive for the addition of atoms (e.g., interstitials). $\epsilon_F$ is the Fermi energy of Ga$_2$O$_3$, defined with respect to the valance band maximum ($\epsilon_{\text{VBM}}$). The $q(\epsilon_{\text{VBM}} + \epsilon_F)$ term therefore accounts for the energy change upon removal or addition of electrons when charge defects are formed.

To remove spurious electrostatic interactions between supercells with charged defects, we include the Freysoldt-Neugebauer-Van de Walle (FNV) correction term $E_{\text{corr}}$. In the FNV scheme, we use a spatially averaged dielectric constant of $\epsilon_0 \sim 10$ [1,23] which includes ionic and electronic screening [24]. There has been some debate, if the electronic dielectric constant $\epsilon_{\text{el}}$ should be used instead for small supercells [25]. However, we observed that $\epsilon_0$ is the correct choice by extrapolating supercells to the infinite supercell limit (see Appendix C). Our findings are in agreement with those of Ingebritsen et al. [24].

All DFT calculations in this work were performed with the all-electron numeric-atom-centered orbital code FHI-AIMS [26–29]. We used the semi-local Perdew-Burke-Ernzerhof (PBE) functional [30] and the Heyd-Scuseria-Ernzerhof hybrid functional (HSE06) [31] to calculate the atomic and electronic structure of β-Ga$_2$O$_3$ and defects therein. PBE calculations are employed as reference to previous work and to test the supercell dependence for charge corrections. For the final defect geometries, we always use the HSE06 functional to avoid spurious delocalization effects in PBE, as observed for, e.g., the oxygen vacancies in TiO$_2$ [32].

We set the fraction of Hartree-Fock exchange in HSE06 to 35%, a value which has been previously used for Ga$_2$O$_3$ [24]. This yields a band gap of 4.95 eV for tight settings in FHI-aims and 4.76 eV for light settings (see below for these two settings), thus providing an acceptable compromise between accuracy and computational cost. Furthermore, we investigated the impact of long-range van der Waals (vdW) corrections based on the Tkatchenko-Scheffler (TS) method [33] on the atomic structure of bulk Ga$_2$O$_3$. Finally, scalar relativistic effects were included by means of the zero-order regular approximation (ZORA) [34].

Considering the computational cost of HSE06 calculations, we carried out most of our calculations with the cheaper “light” basis sets (which usually provide sufficiently converged energy differences) and used results with “tight” basis sets (which can better provide converged absolute energies) as reference. For light settings, we use the tier 1 basis set for oxygen and gallium, but exclude the $f$ function for gallium. For tight settings, we use tier 2 for oxygen and the full tier 1 basis for gallium. Adding tier 2 for gallium did not improve the result with PBE thus the tier 1 basis set for gallium is enough to achieve convergence. A $\Gamma$-centered $2 \times 8 \times 4$ $k$-point mesh was used for the 20-atom monoclinic unit-cell calculations, while for larger supercells (160-atom) we used a $\Gamma$-centered $2 \times 2 \times 2$ $k$-point mesh. In pursuit of open materials science [35], we made the results of all relevant calculations available on the Novel Materials Discovery (NOMAD) repository [36].
III. RESULTS

A. Bulk $\beta$-Ga$_2$O$_3$ and chemical potentials

The optimized geometry of bulk $\beta$-Ga$_2$O$_3$ is presented in Table I for HSE06 and semi-local functionals. Band gaps and formation enthalpies have been included for completeness. The PBE functional overestimates the lattice constants compared to experiment. Van der Waals effects slightly reduce the lattice constants towards better agreement with experiment. Conversely, the HSE06 functional reproduces the experimental geometry well and our results are consistent with those previously reported in the literature \cite{19,21,23,25}.

The HSE06 band structure of $\beta$-Ga$_2$O$_3$ is shown in Fig. 2. The band gap is indirect between the M-point and the Γ-point and has a value of 4.92 eV. The direct gap at the Γ-point is slightly larger (4.95 eV). The fact that indirect transitions are weak makes $\beta$-Ga$_2$O$_3$ effectively a direct band-gap material.

![Figure 2. HSE06 band structure of $\beta$-Ga$_2$O$_3$.](image)

### Table I. Lattice parameters ($a$, $b$, $c$ and $\beta$) of bulk $\beta$-Ga$_2$O$_3$, as well as the band gap ($E_g$) and formation energy ($H_I$) calculated with different DFT functionals. $H_I$ is given in eV per Ga$_2$O$_3$ unit. Also listed are experimental (Exp.) results for the lattice parameters \cite{37} and band gap \cite{11} as reference.

|        | PBE | PBE+TS | HSE06 | Exp. |
|--------|-----|--------|-------|------|
| $a$ [Å] | 12.46 | 12.34  | 12.23 | 12.23 | \cite{37} |
| $b$ [Å] | 3.08  | 3.07   | 3.05  | 3.04  | \cite{37} |
| $c$ [Å] | 5.88  | 5.88   | 5.81  | 5.80  | \cite{37} |
| $\beta$ [°] | 103.7 | 103.9  | 103.7 | 103.7 | \cite{37} |
| $E_g$ [eV] | 1.95  | 2.04   | 4.95  | 4.9   | \cite{11} |
| $H_I$ [eV] | -10.6 | -10.1  | -11.3 | \cite{37} |

We reference the gallium chemical potential $\mu_{\text{Ga}}$ to gallium metal and the oxygen chemical potential $\mu_{\text{O}}$ to the oxygen molecule O$_2$ (see Appendix A for details). The chemical potentials need to be in equilibrium $2\mu_{\text{Ga}} + 3\mu_{\text{O}} = H_{\text{f}}(\text{Ga}_2\text{O}_3)$, which defines the Ga-rich ($\mu_{\text{Ga}} = 0$) and O-rich ($\mu_{\text{O}} = 0$) limits. For the B chemical potential, we use diborane B$_2$H$_6$, which is used as precursor for boron doping e.g. in silicon \cite{58}. The boron chemical potential is defined through the hydrogen chemical potential, which we reference against the hydrogen molecule: $\frac{1}{2} \left( E(\text{B}_2\text{H}_6) - 3E(\text{H}_2) \right)$. Note that we do not vary the hydrogen chemical potential in this study, but keep it fixed. A further constraint on the boron chemical potential is the formation of boron oxide B$_2$O$_3$. The upper bound of the boron chemical potential is therefore $\mu_B \leq \Delta + \mu_{\text{Ga}}$, where $\Delta = \frac{1}{2} \left( H_{\text{f}}(\text{B}_2\text{O}_3) - H_{\text{f}}(\beta-\text{Ga}_2\text{O}_3) \right)$ amounts to -1.12 eV in HSE06. Thus the boron and gallium chemical potentials are linked. Even in the most favorable boron-rich conditions the chemical potential of boron has to be lower than that of gallium.

B. Intrinsic defects

We first investigate intrinsic point defects. We do this not only to validate our calculations against previous studies, but also to study the competition between intrinsic defects and boron defects. We consider vacancy sites and simple interstitials, which we find to be energetically quite stable and thus enough for our assessment of boron defects \cite{24,25}. Intrinsic defects for Ga-rich and O-rich cases are shown in Fig. 3.

The most important transition states of vacancy defects are listed in Table II. The charge transition levels of the oxygen vacancies $\epsilon(+2/0)$ are located deep below the conduction band minimum (CBM). Different coordinations yield slightly different transition states with the four-fold O(III) site being closest to the CBM. For n-type conditions (Fermi energy close to the CBM), the oxygen vacancies are therefore neutral while they would behave as donors for p-type conditions (Fermi energy close to the VBM). Conversely, gallium vacancies act as deep acceptors for most of the Fermi energy range. Here the $\epsilon(−2/−3)$ transition state for the lower coordinated Ga(I) is closer to the CBM than the octahedral Ga(II) state. We note in passing, that the Ga(I) vacancy in the -2 charge state requires a hybrid functional treatment. In the PBE functional the extra electrons do not localize, resulting in a formation energy that is too low.

The interstitial defects are more complex (see Fig. 3). We studied two oxygen interstitials, a split interstitial (O$_{si}$) on the O(I) site and a three-fold coordinated interstitial (O$_i$). For gallium interstitials, we considered two different configurations. In the V$_{Ga}$ interstitial one gallium is removed from the Ga(I)-site and the second Ga(I) moves to an interstitial position with octahedral coordination. In the second configuration (Ga$_i$) we add one gallium atom with octahedral coordination into an interstitial position such that two nearby Ga(I) gallium atoms are pushed away from the interstitial gallium. The

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C. Boron defects

Next we turn to boron point defects. We did initial calculation for neutral defects with the PBE functional, which are shown in Appendix B. PBE and HSE06 give the same formation energy ordering for neutral defects. We therefore scanned a variety of neutral defects with PBE. A clear picture emerges: 4-fold coordinated boron defects are the lowest in energy. We then picked three substitutional defects on Ga-sites with one or two borons and further investigated them with HSE06.

The boron defect geometries are shown in Fig. 4 and the corresponding formation energies in Fig. 5 for three

| Defect  | q/q' | Transition level   |
|---------|------|--------------------|
| O_{si}  | +1/0 | -3.08              |
| O_i     | -1/-2| -1.20              |
| V_{Ga}  | -2/-3| -2.46              |
| V_{Ga}  | -1/-2| -2.73              |
| V_{Ga}  | 0/-1 | -3.00              |
| Ga_i    | +3/+1| -0.69              |

Table II. Transition levels of vacancy defects. All energies (in eV) are given with respect to the conduction band minimum (CBM). The transition level is the energy at which two defect charge states, q and q', are in equilibrium. Reference 24 uses 32% fraction of exact exchange in HSE06 while in Ref. 25 26% exact exchange is used with no range separation.

| Vacancy site | This work | [24] | [25] |
|--------------|-----------|------|------|
| Ga(I)        | -1.65     | -1.76| -1.64|
| Ga(I)        | -2.21     | -2.32| -    |
| Ga(II)       | -2.06     | -2.17| -2.12|
| Ga(II)       | -2.39     | -2.50| -    |
| O(I)         | -1.38     | -1.50| -1.71|
| O(II)        | -2.11     | -2.23| -2.29|
| O(III)       | -1.24     | -1.36| -1.56|

C. Boron defects

Next we turn to boron point defects. We did initial calculation for neutral defects with the PBE functional, which are shown in Appendix B. PBE and HSE06 give the same formation energy ordering for neutral defects. We therefore scanned a variety of neutral defects with PBE. A clear picture emerges: 4-fold coordinated boron defects are the lowest in energy. We then picked three substitutional defects on Ga-sites with one or two borons and further investigated them with HSE06.

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| Defect  | q/q' | Transition level   |
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| O_i     | -1/-2| -1.20              |
| V_{Ga}  | -2/-3| -2.46              |
| V_{Ga}  | -1/-2| -2.73              |
| V_{Ga}  | 0/-1 | -3.00              |
| Ga_i    | +3/+1| -0.69              |
different chemical environments (O-rich, Ga-rich and intermediate conditions \( \mu_{Ga} = \mu_{O} = \frac{1}{2}H_{1}(Ga_{2}O_{23}) \)). Such intermediate conditions are likely closer to the experimental growth conditions than either of the two extreme limits.

Boron preferably incorporates into the tetrahedrally coordinated Ga(I) site. The neutral \( B_{Ga(I)} \) substitutional defect is very stable and does not introduce charge states into the band gap. Boron on the Ga(II) site, \( B_{Ga(II)} \), is not able to maintain the 6-fold coordination of the substituted gallium due to its much smaller ionic size. This leads to a larger relaxation of the surrounding atoms such that \( B_{Ga(II)} \) becomes 3-fold coordinated and introduces a dangling bond on one of the neighboring oxygen atoms. In this site, boron can therefore act as donor with a \( \varepsilon (+1/0) \) transition state at 1.29 eV above the VBM.

Another interesting boron defect is the two-boron complex on the Ga(II) site (2\( B_{Ga(II)} \)) shown in Fig. 4. Each boron is 4-fold coordinated, which makes the formation energy competitive to the other two boron defects we discussed. However, since two boron atoms replace one gallium atom in this defect, the constraint on the boron chemical potential (\( \mu_{B} < \mu_{Ga} \)) makes it hard for this defect to compete with gallium vacancies. For this reason, it is unlikely that this two-boron defect complex forms without forming \( B_{2}O_{3} \) first. Similar two boron structures were constructed on the Ga(I) and interstitial sites but they were not 4-fold coordinated thus resulting in considerably higher formation energies.

Next, we address the range of boron chemical potential, in which boron defects form preferentially. In Fig. 5, the boron chemical potential is as boron rich as possible without forming \( B_{2}O_{3} \) (\( \mu_{B} = \Delta + \mu_{Ga} \)), where \( \Delta = \varepsilon \left( E_{i}(B_{2}O_{3}) - E_{i}(\beta-Ga_{2}O_{3}) \right) \). The range of feasible boron chemical potential depends on the competition between gallium vacancies and boron substitutionals, which in turn depends on the Fermi-level position during growth.

Clearly the incorporation of neutral borons on gallium sites, especially Ga(I), is the most preferable way of doping. Neutral boron defects are preferable as we are not interested in making electronically active defects but incorporating boron as a neutron active material.

In experimental crystal growth, the Fermi level is expected to be pinned deep below the CBM \([24,25]\) (e.g. 0.8 ~ 2.6 eV below CBM in \([24]\)). Under such conditions, boron incorporation is relatively likely in the intermediate chemical potential conditions depicted in the middle panel of Fig. 5. Also in oxygen-rich conditions, boron can be incorporated, but it starts to compete with gallium vacancies. Gallium-rich growth conditions are not favorable for B implantation. To make a more refined assessment on B incorporation in \( Ga_{2}O_{3} \) one would also have to consider the role of hydrogen \([24,39]\), with which B competes \([40]\).

### IV. CONCLUSION

We have investigated boron related point defects in \( \beta-Ga_{2}O_{3} \) with DFT for a possible use of the material in solid-state neutron detectors. We found that boron preferably incorporates onto 4-fold coordinated gallium sites. Such boron defects are electronically neutral and do not introduce trap states in the band gap. Larger boron complexes have similar formation energies, but are unlikely to form due to competition with the \( B_{2}O_{3} \) formation. Intermediate growth regimes between the Ga-rich and O-rich limits are most conducive to boron incorporation.

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### Appendix A: Chemical potentials

For completeness, we report the total energies used for calculating the chemical potentials in Table [IV]. For gallium, we used gallium metal in the orthorhombic structure with 8 atoms per unit cell as reference. The calculations were performed with a \( 8 \times 8 \times 8 \) \( \Gamma \)-centered k-point mesh. Oxygen is referenced to the oxygen molecule \( \frac{1}{2}E(O_{2}) \). For boron oxide \( (B_{2}O_{3}) \), we took the \( \alpha \)-phase with 15 atoms per unit cell. The calculations were performed with a \( 4 \times 4 \times 4 \) \( \Gamma \)-centered k-point mesh. [11].

| System    | Energy (eV) | System    | Energy (eV) |
|-----------|-------------|-----------|-------------|
| Ga        | -53183.059  | \( B_{2}O_{3} \) | -7505.521   |
| O         | -2046.547   | \( H_{2} \)    | -31.834     |
| \( Ga_{2}O_{3} \) | -112515.856 | \( B_{2}H_{6} \) | -1449.042   |

Table IV. Reference systems used in the calculations of the chemical potentials. For each system the energy is given per formula unit except for gallium and oxygen where it is given per atom.
Figure 4. Structure of the boron defect sites in Ga$_2$O$_3$ supercell: (a) Boron on Ga(II)-site with three-fold coordination, (b) boron on Ga(I)-site with four-fold coordination c) two 4-fold coordinated boron atoms on the Ga(II) site.

Figure 5. Defect formation energies $E_f$ for multiple intrinsic defects and the most important boron defects. The chemical potential of Gallium is $\mu_{\text{Ga}} = \frac{1}{2} H_f(\text{Ga}_2\text{O}_3)$ for the intermediate case.

Appendix B: Boron defects with the PBE functional

In Table 5 we tabulate neutral defects calculated with the PBE and HSE06 functional. The formation energies are given for the Ga-rich ($\mu_{\text{Ga}} = 0$ eV) and boron rich ($\mu_{\text{B}} = -1.17$ eV) limit. The gallium and oxygen vacancies are listed for reference to demonstrate that they have the same energetic ordering as neutral vacancies with the HSE06 functional.

Boron defects B$_{\text{Ga(I)}}$ and B$_{\text{Ga(II)}}$ are substitutional defects on Ga-sites. More complex substitutional defects are 2B$_{\text{Ga(II)}}$, 2B$_{\text{Ga(I)}}$ and 3B – (2Ga(II)), in which two or three boron atoms replace Ga atoms. The B$_i$ interstitial has a lower formation energy than the (2B) – Ga$_i$ interstitial, in which a gallium atom moves to an interstitial site and the vacant Ga-site is filled with two substitutional borons.

Appendix C: Electrostatic corrections

We verified the FNV corrections for the Ga(II) vacancy in two charge states by an explicit supercell convergence with the PBE functional. The results are shown in Fig. 6. The structures are multiples of the unit cell, which have been relaxed after the removal of one gallium in the Ga(II)-site. For The FNV correction we use a dielectric constant $\varepsilon_0$ of 10. Applying the FNV correction results in horizontal lines with formation energies that are independent of the supercell size.

Appendix D: Interstitial defects in $\beta$-Ga$_2$O$_3$

In Fig. 7 we show the atomic configurations for the interstitial defects. The structure of vacancies is straightforward and therefore not shown for brevity.
Table V. The formation energies (eV) of neutral Boron defects and vacancies computed with PBE and HSE06 functional. See text for details.

| Defect          | $E_f$ (PBE) | $E_f$ (HSE06) |
|-----------------|-------------|---------------|
| $V_{Ga(I)}$     | 9.483       | 9.825         |
| $V_{Ga(II)}$    | 9.597       | 10.755        |
| $V_{O(I)}$      | 1.085       | 4.824         |
| $V_{O(II)}$     | 0.607       | 4.262         |
| $V_{O(III)}$    | 1.322       | 5.089         |
| $B_{Ga(I)}$     | -0.196      | 1.240         |
| $B_{Ga(II)}$    | 0.628       | 2.143         |
| (2B)$_{Ga(II)}$ | 2.440       | 3.392         |
| $B_i$           | 2.841       | -             |
| (2B)$_{Ga(I)}$  | 3.285       | -             |
| (3B) – (2Ga(II))| 4.344       | -             |
| (2B) – Ga$_i$   | 4.965       | -             |

Figure 6. Defect formation energies for $V_{Ga(II)}$ in the $-3$ charge state $-3$ (upper) and the $-2$ charge state (lower) as a function of the inverse super cell volume. Defect formation energies (symbols) are calculated for supercells of different sizes with and without the FNV correction. Lines are linear fits to the data.
Figure 7. Atomic configurations of four different interstitials. The interstitials are marked with light blue while important deformations near the interstitial are marked with orange. From left to right: Oxygen split interstitial $O_{Si}$, oxygen interstitial $O_{i}$ and gallium interstitial $Ga_{i}$ with two gallium atoms in orange which have moved from Ga(I)-sites. Finally, on the right gallium interstitial $V^{Ga}_{Ga}$ which is surrounded by two Ga(II)-sites and two empty Ga(I)-sites.
