Electronic Supplementary Information:

Ab initio approach on the asymmetric stacking of GaAs <111> nanowires grown by vapor-solid method

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Chemical potential (T, P_{As})

The chemical potential of bulk solid, $\mu_{(Solid)}(T,P)$, was considered to be the Helmholtz energy ($F=E-TS_{vib}$) per formula unit, since the PV contribution to the Gibbs free energy ($G=F+PV$) is negligible in the low pressure vapor–solid system described in this study. The chemical potential of gas phase, $\mu_{(Gas)}(T,P)$, was calculated by using statistical mechanics[1] in which the thermodynamic properties of molecule are defined by the molecular partition functions of each degree of freedom (e.g., translational, rotational, vibrational, and electronic motions). The detailed procedure to calculate the chemical potentials of bulk solid and gas phase is described in the authors' previous work.[2] Figure S1 shows the calculated chemical potentials of nucleus ($\mu_{n(GaAs)}$) and sources ($\mu_{s(Ga)}$ and $\mu_{s(As)}$) in the most stable phase under given T at P_{As} of 3×10^{-9} atm: zinc-blende for n(GaAs), orthorhombic for s(Ga), and gas mixture consisting of As_2 and As_4 molecules for s(As). These values were used to obtain the T–P dependent incorporation energy: $\Delta\mu_{sn} = \mu_{n(GaAs)} - \mu_{s(Ga)} - \mu_{s(As)}$.

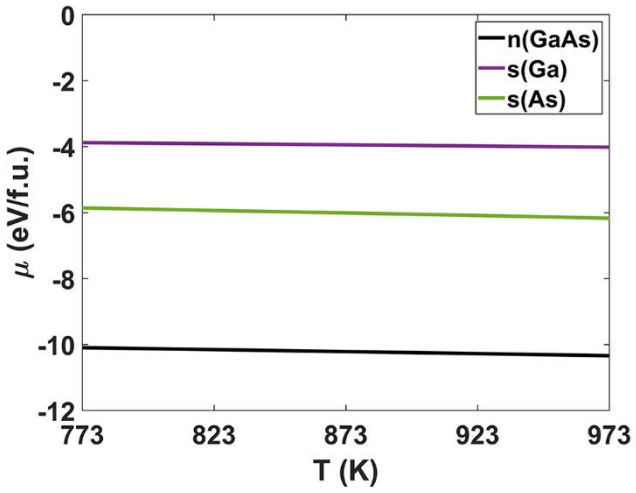

Figure S1. Chemical potentials of GaAs nucleus (n), Ga source (s), and As source (s), as a function of T at P_{As} of 3×10^{-9} atm.

Surface energy (T, P_{As})

The T–P dependent surface energies for relevant reconstructions of the (110), (111)A, and (111)B surfaces were calculated following our previous works:[3,4]

$$\gamma^{elec} = \frac{\left(E_{surf}^{elec}\right) - N_{Ga}(E_{GaAs(bulk)}^{elec}) - (N_{As} - N_{Ga})(E_{As(GaAs)}^{elec})}{A} - (\gamma_H + \alpha) \quad \text{(S1)}$$

$$\Delta\gamma^{vib} = \frac{\left(F_{surf}^{vib}\right) - N_{Ga}(F_{GaAs(bulk)}^{vib}) - (N_{As} - N_{Ga})(F_{As(GaAs)}^{vib})}{A} \quad \text{(S2)}$$

where, γ^{elec} and $\Delta\gamma^{vib}$ are the electronic and vibrational surface energy, respectively; E_{surf}^{elec}, $E_{GaAs(bulk)}^{elec}$, and $E_{As(GaAs)}^{elec}$ are the electronic energies of the slab consisting of the unreconstructed bottom and reconstructed top surfaces, bulk GaAs, and As in bulk GaAs, respectively; $\gamma_H + \alpha$ is the electronic surface energy of the unreconstructed bottom surface whose dangling bonds were saturated by pseudo-hydrogen (the number of valence electron of hydrogen is 1.25 for Ga–H bond and 0.75 for As–H bond); F_{surf}^{vib}, $F_{GaAs(bulk)}^{vib}$, and $F_{As(GaAs)}^{vib}$ are the vibrational energies of the atoms at the reconstructed top three layers, bulk GaAs, and As in bulk GaAs, respectively; and N_{Ga}, N_{As}, and A are the numbers of Ga and As atoms and the surface area of the slab, respectively. The convergence of surface energy with respect to the slab geometry and procedures to obtain $\gamma_H + \alpha$ are described in detail in the Supplementary Information of the previous work.[4]

γ^{elec} is generally obtained as a function of the chemical potential of As in the bulk GaAs, $\mu_{As(GaAs)}$, due to the stoichiometry imbalance at the surface reconstruction as shown in Fig. S2. The atomic structures of each reconstruction are presented in the Supplementary Information of the previous work.[3] In those figures, stable reconstructions with low electronic surface energy are highlighted for each surface.

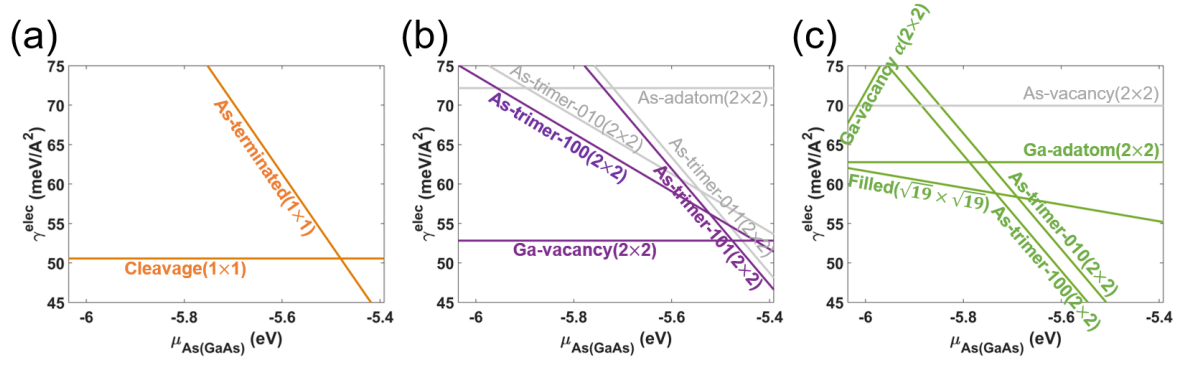

Figure S2. Calculated electronic surface energy of GaAs (a) (110), (b) (111)A, and (c) (111)B surfaces as a function of the chemical potential of As in bulk GaAs.

By assuming the chemical equilibrium between the surface and surrounding gas, $\mu_{As(GaAs)}$=$\mu_{As(Gas)}$, $\gamma^{elec}(\mu_{As(GaAs)})$ could be converted to $\gamma^{elec}(T, P_{As})$, called implicit T dependence,[5] because the T–P dependent chemical potential in the gas phase ($\mu_{As(Gas)}(T, P_{As})$) can be calculated using statistical mechanics as mentioned above. In this study, the As gas was considered to be a gas mixture consisting of As_2 and As_4 molecules in equilibrium:

$$\mu_{As(Gas)} = \frac{1}{2}\mu_{As_2(Gas)} = \frac{1}{4}\mu_{As_4(Gas)} \quad \text{(S3)}$$

$$P_{As} = P_{As_2} + P_{As_4} \quad \text{(S4)}$$

where, $\mu_{As(Gas)}$, $\mu_{As_2(Gas)}$, and $\mu_{As_4(Gas)}$ are the chemical potentials of the As gas mixture in equilibrium, As_2, and As_4 molecule, respectively; and P_{As}, P_{As_2}, and P_{As_4} indicate the total As pressure, partial pressure of As_2, and As_4 molecule, respectively. Figure S3 shows $\mu_{As(Gas)}$ as a function of T at three different P_{As} and Fig. S4 presents the converted γ^{elec} as a function of T at P_{As} of 3×10^{-9} atm.

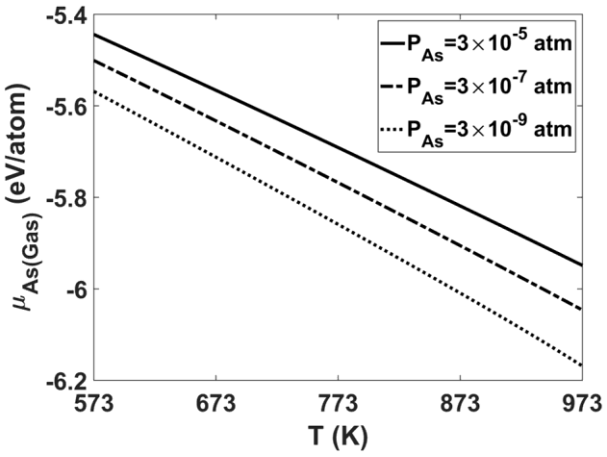

Figure S3. Calculated chemical potential of the As gas mixture in equilibrium as a function of T at P_{As} of 3×10^{-5}, 3×10^{-7}, and 3×10^{-9} atm.

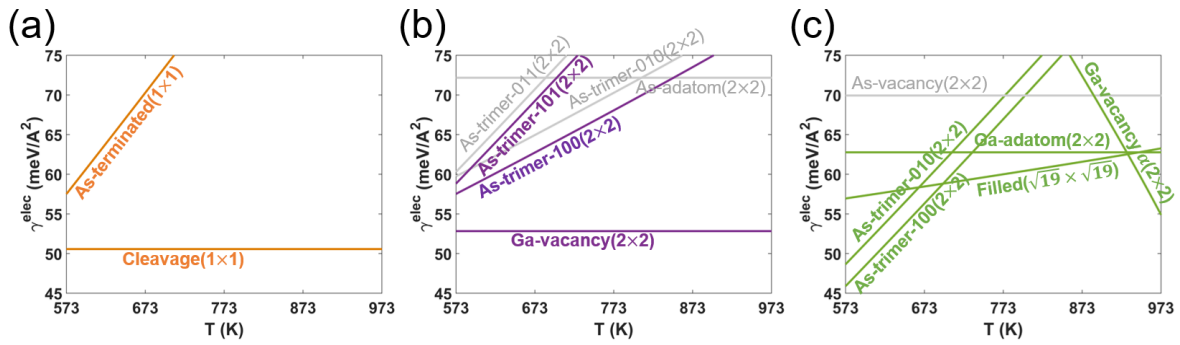

Figure S4. Electronic surface energy of GaAs (a) (110), (b) (111)A, and (c) (111)B surfaces as a function of T at P_{As} of 3×10^{-9} atm.

In addition, the vibrational surface energy ($\Delta\gamma^{vib}$), called explicit T-dependence,[5] can be obtained as a function of T, as all the vibrational energies (F^{vib}) and following $\Delta\gamma^{vib}$ in Eq. (S2) are functions of T:

$$F^{vib} = \frac{1}{N_k}\sum_{k\in BZ}\sum_{i=1}^{M}\{\frac{\hbar w_i(k)}{2} + k_B T \ln\left(1 - e^{-\frac{\hbar w_i(k)}{k_B T}}\right)\} \quad \text{(S5)}$$

where, N_k and M are the numbers of k-points and phonon modes, respectively; $\hbar$ and k_B are the reduced Planck constant and the Boltzmann constant, respectively; and $w_i(k)$ is the angular frequency of i-th phonon mode at k-point in the Brillouin zone (BZ). Bulk phonon density of state (DOS) of GaAs (Fig. S5) was obtained using PHONOPY program,[6,7] and integrated to calculate $F^{vib}_{GaAs(bulk)}$ and $F^{vib}_{As(GaAs)}$ in Eq. (S2) using Eq. (S5).

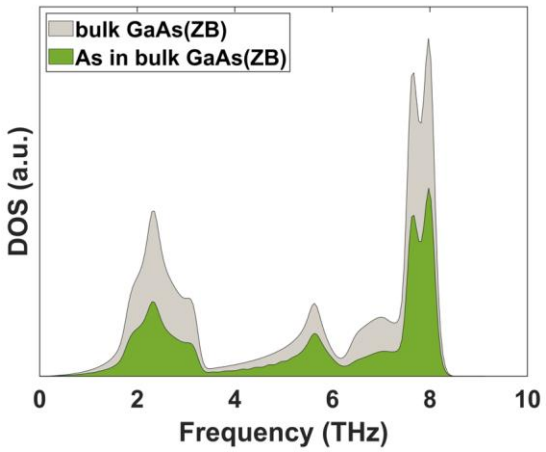

Figure S5. The total phonon DOS of zinc-blende (ZB) GaAs (gray area) and corresponding partial phonon DOS of As in the bulk GaAs (green area).

On the other hand, F^{vib}_{surf} in Eq. (S2) was calculated by surface phonon DOS, which was obtained by dynamical matrix of 21×21 k-points sampled at equal intervals on the surface BZ. The dynamical matrix was calculated by perturbing the atoms at the top three layers, because the bonding state and vibration of the atoms at deeper than the top three layers are almost identical to those of the atoms in bulk state.[3] For both the bulk and surface phonon calculations, the finite displacement method within the harmonic approximation was employed. Since the situation described in this study is the vapor–solid system at a low pressure, the volume dependence of the vibrational frequency was neglected.

Then, the total surface energy, sum of electronic and vibrational surface energy ($\gamma = \gamma^{elec} + \Delta\gamma^{vib}$), can be obtained as a function of T and P_{As} as shown in Fig. S6. Compared with Fig. S4, the surface energy is lowered by 5~10 meV/Å^2 and the amount of the decrease is different for each reconstruction. This is because the surface phonon and its difference with bulk phonon are various, caused by the different bonding state of each reconstruction. The surface phonon DOSs of relevant reconstructions will be shown in Figs. S8-S10 with bulk phonon DOS for comparison.

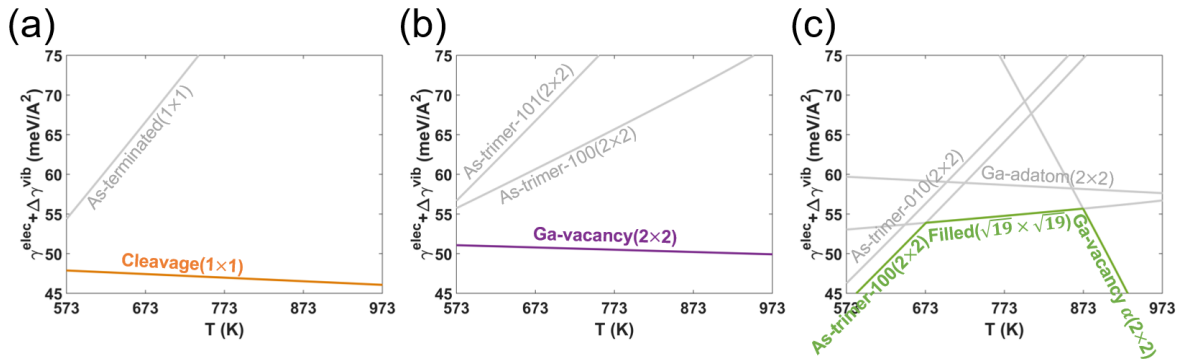

Figure S6. Calculated total surface energy of GaAs (a) (110), (b) (111)A, and (c) (111)B surfaces as a function of T at P_{As} of 3×10^{-9} atm. The lowest surface energy line is highlighted along the most stable reconstructions for each surface.

(111)A and (111)B surfaces without reconstruction

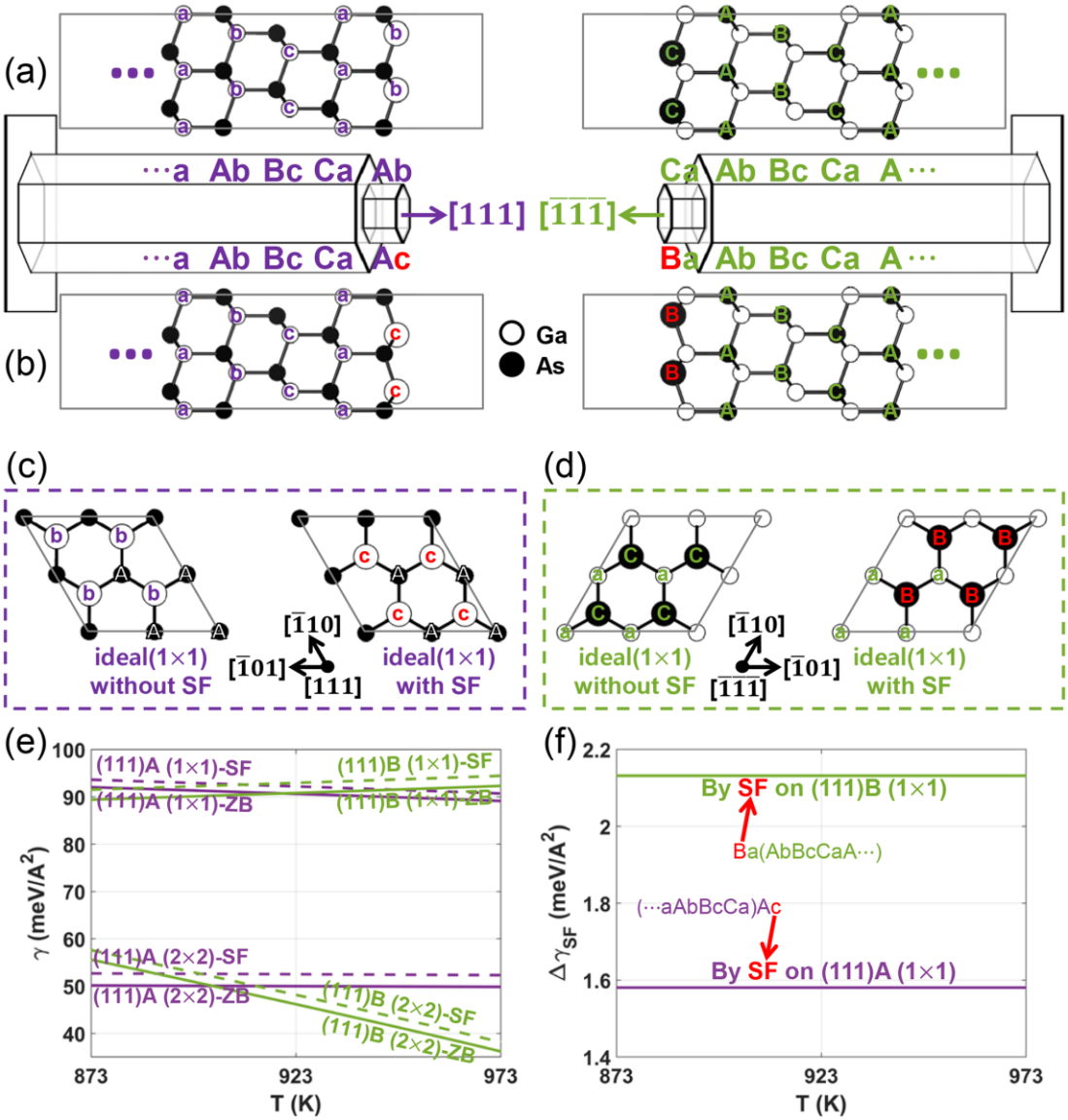

Figure S7. Side views of unreconstructed GaAs (111)A and (111)B surfaces (a) without, and (b) with SF at the surface topmost layer. (c) Top views of the unreconstructed (111)A, and (d) (111)B without, and with SF. Corresponding (e) surface energy ($\gamma=\gamma^{elec}+\gamma^{vib}$) at P_{As} of 3×10^{-9} atm without (solid line), and with (dashed line) SF on the topmost layer. For comparison, the surface energy of (2×2) reconstructions is also presented, which is identical to Fig. 4 in manuscript. (f) The amount of surface energy increase by SF in the unreconstructed (111)A and (111)B surfaces.

Surface phonon DOSs

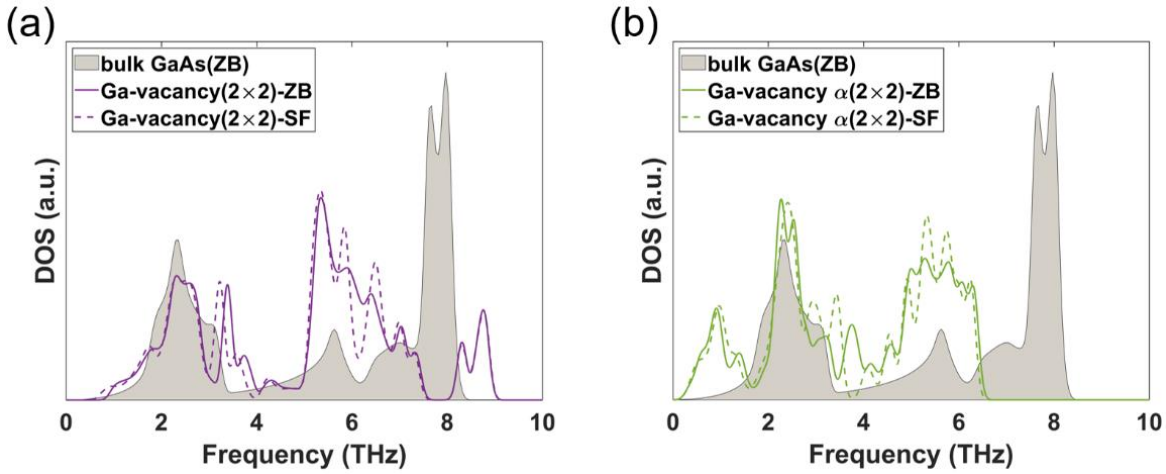

Figure S8. Surface phonon DOSs of (a) GaAs (111)A Ga-vacancy(2×2), and (b) (111)B Ga-vacancy α(2×2) without (solid line), and with (dashed line) stacking fault (SF) at the surface topmost layer. The shaded area corresponds to the bulk phonon DOS of zinc-blende (ZB) GaAs. Note that the calculated frequency of As_2 molecule is 13.38 THz; and that of As_4 molecule is (6.35, 6.35, 8.08, 8.08, 8.08, 10.85) THz.

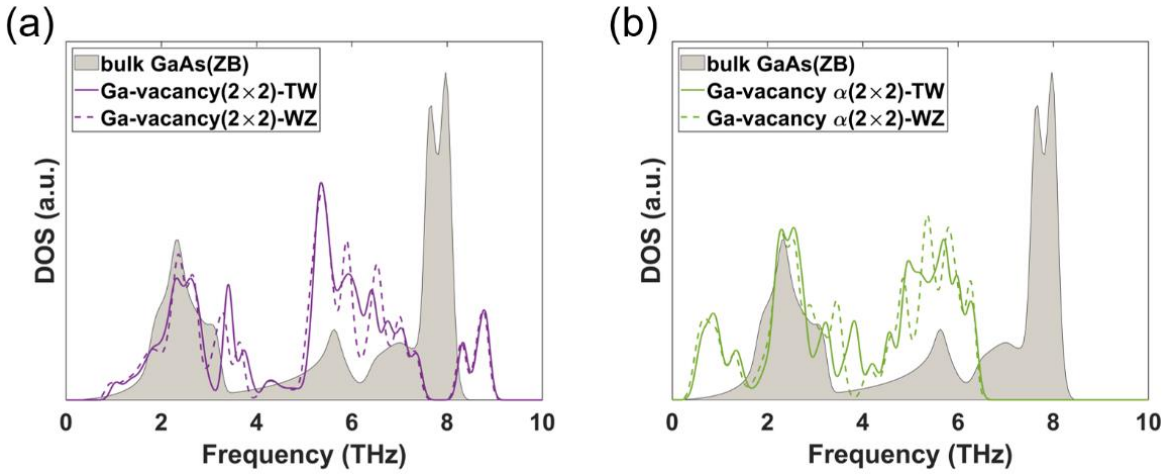

Figure S9. Surface phonon DOSs of (a) GaAs (111)A Ga-vacancy(2×2), and (b) (111)B Ga-vacancy α(2×2) with TW- (solid line) and WZ- (dashed line) stacking at the topmost layers. The shaded area corresponds to the bulk phonon DOS of ZB GaAs.

Chemical potential and surface energy of wurtzite phase

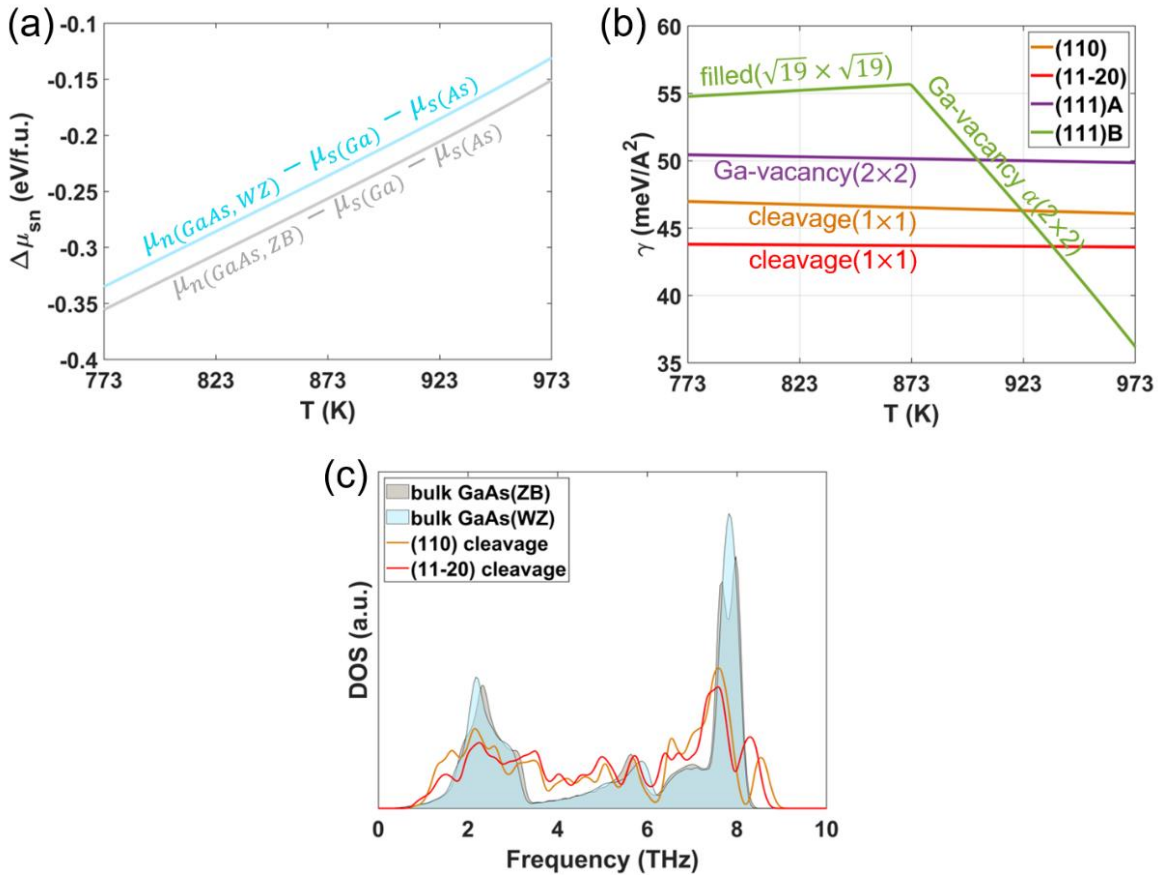

Figure S10. (a) Change in chemical potential by the incorporation of source into nucleus of ZB (gray) and WZ phase (sky blue). (b) Surface energies of the most stable reconstructions including WZ $(11\bar{2}0)$ cleavage as a function of T at a fixed P_{As} (=P_{As2}+P_{As4}) of 3×10^{-9} atm. (c) Surface phonon DOSs of (110) cleavage (dark yellow line) and $(11\bar{2}0)$ cleavage (red line). The shaded area corresponds to the bulk phonon DOSs of ZB (gray) and WZ (sky blue).

References

[1] D. A. McQuarrie, *Statistical Mechanics*, University Science Books, California, 2000.

[2] I. W. Yeu, J. Park, G. Han, C. S. Hwang and J.-H. Choi, *Sci. Rep.*, 2017, **7**, 10691.

[3] I. W. Yeu, G. Han, J. Park, C. S. Hwang and J.-H. Choi, *Sci. Rep.*, 2019, **9**, 1127.

[4] I. W. Yeu, G. Han, J. Park, C. S. Hwang and J.-H. Choi, *Appl. Surf. Sci.*, 2019, **497**, 143740.

[5] M. Valtiner, M. Todorova, G. Grundmeier and J. Neugebauer, *Phys. Rev. Lett.*, 2009, **103**, 065502.

[6] A. Togo, F. Oba and I. Tanaka, *Phys. Rev. B*, 2008, **78**, 134106.

[7] A. Togo, L. Chaput, I. Tanaka and G. Hug, *Phys. Rev. B*, 2010, **81**, 174301.

Cartesian coordinates and DFT energies.

For the solid-vapor-surface structures relevant to this work, the relaxed coordinates in CIF format and corresponding energies are presented in the following order:

1. Solid
   - **1-1.** GaAs(zinc-blende)
   - **1-2.** GaAs(wurtzite)
   - **1-3.** Ga(orthorhombic)
2. Vapor
   - **2-1.** As_2
   - **2-2.** As_4
3. Surface slab of GaAs
   - **3-1.** (110) cleavage(1×1)
   - **3-2.** $(11\bar{2}0)$ cleavage(1×1)
   - **3-3.** (111)A Ga-vacancy(2×2)-ZB
   - **3-4.** (111)A Ga-vacancy(2×2)-SF
   - **3-5.** (111)A Ga-vacancy(2×2)-TW
   - **3-6.** (111)A Ga-vacancy(2×2)-WZ
   - **3-7.** (111)B filled(√19×√19)
   - **3-8.** (111)B Ga-vacancy α(2×2)-ZB
   - **3-9.** (111)B Ga-vacancy α(2×2)-SF
   - **3-10.** (111)B Ga-vacancy α(2×2)-TW
   - **3-11.** (111)B Ga-vacancy α(2×2)-WZ

1-1. GaAs(zinc-blende); Energy: –38.434660 eV (–1.4124478 Hartrees)

```
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_cell_length_b                         5.60929
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_cell_angle_beta                       90
_cell_angle_gamma                      90

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loop_
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   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
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   Ga2     1.0     0.000000     0.500000     0.500000     Biso    1.000000 Ga
   Ga3     1.0     0.500000     0.000000     0.500000     Biso    1.000000 Ga
   Ga4     1.0     0.500000     0.500000     0.000000     Biso    1.000000 Ga
   As1     1.0     0.250000     0.250000     0.250000     Biso    1.000000 As
   As2     1.0     0.750000     0.750000     0.250000     Biso    1.000000 As
   As3     1.0     0.750000     0.250000     0.750000     Biso    1.000000 As
   As4     1.0     0.250000     0.750000     0.750000     Biso    1.000000 As
```

1-2. GaAs(wurtzite); Energy: –19.170088 eV (–0.7044878 Hartrees)

```
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   _atom_site_fract_z
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   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
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   Ga2     1.0     0.333333     0.666667     0.501575     Biso    1.000000 Ga
   As1     1.0     0.666667     0.333333     0.375425     Biso    1.000000 As
   As2     1.0     0.333333     0.666667     0.875425     Biso    1.000000 As
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1-3. Ga(orthorhombic); Energy: –28.575456 eV (–1.0501287 Hartrees)

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loop_
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   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
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   Ga3        1.0     0.000000     0.655792     0.415005     Biso   1.000000 Ga
   Ga4        1.0     0.500000     0.155792     0.415005     Biso   1.000000 Ga
   Ga5        1.0     0.000000     0.344208     0.584995     Biso   1.000000 Ga
   Ga6        1.0     0.500000     0.844208     0.584995     Biso   1.000000 Ga
   Ga7        1.0     0.000000     0.844208     0.915005     Biso   1.000000 Ga
   Ga8        1.0     0.500000     0.344208     0.915005     Biso   1.000000 Ga
```

2-1. As_2; Energy: –8.0984290 eV (–0.2976118 Hartrees)

```
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_cell_length_c                         17.45988
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```

2-2. As_4; Energy: –19.519949 eV (–0.7173450 Hartrees)

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_cell_length_c                         17.45988
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_cell_angle_gamma                        90

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   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
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   As2        1.0     0.567667     0.499263     0.575192     Biso    1.000000 As
   As3        1.0     0.499262     0.567667     0.674808     Biso    1.000000 As
   As4        1.0     0.499256     0.428816     0.673369     Biso    1.000000 As
```

3-1. (110) cleavage(1×1); Energy: –91.307366 eV (–3.3554841 Hartrees)

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loop_
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   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Ga1        1.0     0.000000     0.000000     0.000000     Biso    1.000000 Ga
   Ga2        1.0     0.500000     0.500000     0.062500     Biso    1.000000 Ga
   Ga3        1.0     0.000000     0.000000     0.125000     Biso    1.000000 Ga
   Ga4        1.0     0.500000     0.500000     0.187500     Biso    1.000000 Ga
   Ga5        1.0     0.002574     0.000000     0.250101     Biso    1.000000 Ga
```

```
Ga6     1.0     0.506334     0.500000     0.312961     Biso    1.000000 Ga
Ga7     1.0     0.006718     0.000000     0.374560     Biso    1.000000 Ga
Ga8     1.0     0.513583     0.500000     0.440353     Biso    1.000000 Ga
Ga9     1.0     0.935973     0.000000     0.486000     Biso    1.000000 Ga
As1     1.0     0.750000     0.500000     0.000000     Biso    1.000000 As
As2     1.0     0.250000     0.000000     0.062500     Biso    1.000000 As
As3     1.0     0.750000     0.500000     0.125000     Biso    1.000000 As
As4     1.0     0.250000     0.000000     0.187500     Biso    1.000000 As
As5     1.0     0.753245     0.500000     0.249968     Biso    1.000000 As
As6     1.0     0.255987     0.000000     0.312177     Biso    1.000000 As
As7     1.0     0.754452     0.500000     0.375828     Biso    1.000000 As
As8     1.0     0.262065     0.000000     0.437173     Biso    1.000000 As
As9     1.0     0.727124     0.500000     0.507786     Biso    1.000000 As
H11     1.0     0.163606     0.000000     0.960122     Biso    1.000000 H1
H.1     1.0     0.583117     0.500000     0.960681     Biso    1.000000 H.
```

3-2. (11$\bar{2}$0) cleavage(1×1); Energy: –182.47448 eV (–6.7058140 Hartrees)

```
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_cell_length_c                         31.61646
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loop_
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   _atom_site_fract_y
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   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Ga1     1.0     0.001575     0.666667     0.000000     Biso    1.000000 Ga
   Ga2     1.0     0.501575     0.333333     0.000000     Biso    1.000000 Ga
   Ga3     1.0     0.501575     0.833333     0.062500     Biso    1.000000 Ga
   Ga4     1.0     0.001575     0.166667     0.062500     Biso    1.000000 Ga
   Ga5     1.0     0.001575     0.666667     0.125000     Biso    1.000000 Ga
   Ga6     1.0     0.501575     0.333333     0.125000     Biso    1.000000 Ga
   Ga7     1.0     0.001575     0.166667     0.187500     Biso    1.000000 Ga
   Ga8     1.0     0.501575     0.833333     0.187500     Biso    1.000000 Ga
   Ga9     1.0     0.000392     0.667103     0.250150     Biso    1.000000 Ga
   Ga10    1.0     0.500392     0.332897     0.250150     Biso    1.000000 Ga
   Ga11    1.0    -0.002825     0.168951     0.313094     Biso    1.000000 Ga
   Ga12    1.0     0.497175     0.831049     0.313094     Biso    1.000000 Ga
   Ga13    1.0    -0.004889     0.668227     0.374935     Biso    1.000000 Ga
   Ga14    1.0     0.495111     0.331773     0.374935     Biso    1.000000 Ga
   Ga15    1.0    -0.006575     0.174905     0.440311     Biso    1.000000 Ga
   Ga16    1.0     0.493425     0.825095     0.440311     Biso    1.000000 Ga
   Ga17    1.0     0.034816     0.614559     0.485647     Biso    1.000000 Ga
   Ga18    1.0     0.534816     0.385441     0.485647     Biso    1.000000 Ga
   As1     1.0     0.375425     0.666667     0.000000     Biso    1.000000 As
   As2     1.0     0.875425     0.333333     0.000000     Biso    1.000000 As
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As3	1.0	0.875425	0.833333	0.062500	Biso	1.000000 As
As4	1.0	0.375425	0.166667	0.062500	Biso	1.000000 As
As5	1.0	0.375425	0.666667	0.125000	Biso	1.000000 As
As6	1.0	0.875425	0.333333	0.125000	Biso	1.000000 As
As7	1.0	0.375425	0.166667	0.187500	Biso	1.000000 As
As8	1.0	0.875425	0.833333	0.187500	Biso	1.000000 As
As9	1.0	0.374491	0.666240	0.250035	Biso	1.000000 As
As10	1.0	0.874491	0.333760	0.250035	Biso	1.000000 As
As11	1.0	0.371173	0.164760	0.312378	Biso	1.000000 As
As12	1.0	0.871173	0.835240	0.312378	Biso	1.000000 As
As13	1.0	0.370160	0.666834	0.375841	Biso	1.000000 As
As14	1.0	0.870160	0.333166	0.375841	Biso	1.000000 As
As15	1.0	0.369240	0.161872	0.437945	Biso	1.000000 As
As16	1.0	0.869240	0.838128	0.437945	Biso	1.000000 As
As17	1.0	0.377711	0.683193	0.506897	Biso	1.000000 As
As18	1.0	0.877711	0.316807	0.506897	Biso	1.000000 As
H11	1.0	0.921858	0.775439	0.959776	Biso	1.000000 H1
H12	1.0	0.421858	0.224561	0.959776	Biso	1.000000 H1
H.1	1.0	0.959444	0.220963	0.960774	Biso	1.000000 H.
H.2	1.0	0.459444	0.779037	0.960774	Biso	1.000000 H.

3-3. (111)A Ga-vacancy(2×2)-ZB; Energy: –195.90990 eV (–7.1995566 Hartrees)

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_cell_length_b                         7.93273
_cell_length_c                         29.14671
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Ga1     1.0     0.000000     0.000000     0.000000     Biso    1.000000 Ga
   Ga2     1.0     0.500000     0.500000     0.000000     Biso    1.000000 Ga
   Ga3     1.0     0.500000     0.000000     0.000000     Biso    1.000000 Ga
   Ga4     1.0     0.000000     0.500000     0.000000     Biso    1.000000 Ga
   Ga5     1.0     0.333333     0.666667     0.111111     Biso    1.000000 Ga
   Ga6     1.0     0.833333     0.666667     0.111111     Biso    1.000000 Ga
   Ga7     1.0     0.833333     0.166667     0.111111     Biso    1.000000 Ga
   Ga8     1.0     0.333333     0.166667     0.111111     Biso    1.000000 Ga
   Ga9     1.0     0.666611     0.333305     0.222114     Biso    1.000000 Ga
   Ga10    1.0     0.166695     0.833389     0.222114     Biso    1.000000 Ga
   Ga11    1.0     0.166695     0.333306     0.222114     Biso    1.000000 Ga
   Ga12    1.0     0.666667     0.833333     0.222433     Biso    1.000000 Ga
   Ga13    1.0     0.000949     0.000474     0.334932     Biso    1.000000 Ga
   Ga14    1.0     0.499526     0.499051     0.334932     Biso    1.000000 Ga
   Ga15    1.0     0.499526     0.000474     0.334932     Biso    1.000000 Ga
```

Ga16	1.0	0.000000	0.500000	0.332434	Biso	1.000000 Ga
Ga17	1.0	0.359613	0.679806	0.420754	Biso	1.000000 Ga
Ga18	1.0	0.820194	0.679806	0.420754	Biso	1.000000 Ga
Ga19	1.0	0.820194	0.140387	0.420754	Biso	1.000000 Ga
As1	1.0	0.000000	0.000000	0.083333	Biso	1.000000 As
As2	1.0	0.000000	0.500000	0.083333	Biso	1.000000 As
As3	1.0	0.500000	0.000000	0.083333	Biso	1.000000 As
As4	1.0	0.500000	0.500000	0.083333	Biso	1.000000 As
As5	1.0	0.333333	0.666667	0.194444	Biso	1.000000 As
As6	1.0	0.333333	0.166667	0.194444	Biso	1.000000 As
As7	1.0	0.833333	0.166667	0.194444	Biso	1.000000 As
As8	1.0	0.833333	0.666667	0.194444	Biso	1.000000 As
As9	1.0	0.665870	0.332935	0.305337	Biso	1.000000 As
As10	1.0	0.666667	0.833333	0.305832	Biso	1.000000 As
As11	1.0	0.167065	0.332935	0.305337	Biso	1.000000 As
As12	1.0	0.167065	0.834129	0.305337	Biso	1.000000 As
As13	1.0	0.044843	0.022422	0.419562	Biso	1.000000 As
As14	1.0	0.000000	0.500000	0.417565	Biso	1.000000 As
As15	1.0	0.477578	0.022422	0.419562	Biso	1.000000 As
As16	1.0	0.477578	0.455156	0.419562	Biso	1.000000 As
As17	1.0	0.166667	0.333333	0.972222	Biso	1.000000 As
As18	1.0	0.166667	0.833333	0.972222	Biso	1.000000 As
As19	1.0	0.666667	0.833333	0.972222	Biso	1.000000 As
As20	1.0	0.666667	0.333333	0.972222	Biso	1.000000 As
H.1	1.0	0.666667	0.333333	0.918783	Biso	1.000000 H.
H.2	1.0	0.166667	0.833333	0.918783	Biso	1.000000 H.
H.3	1.0	0.666667	0.833333	0.918783	Biso	1.000000 H.
H.4	1.0	0.166667	0.333333	0.918783	Biso	1.000000 H.

3-4. (111)A Ga-vacancy(2×2)-SF; Energy: –195.73816 eV (–7.1932453 Hartrees)

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_chemical_name_common                  '111A Ga-vacancy-SF'
_cell_length_a                         7.93273
_cell_length_b                         7.93273
_cell_length_c                         29.14671
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Ga1     1.0     0.000000     0.000000     0.000000     Biso    1.000000 Ga
   Ga2     1.0     0.500000     0.500000     0.000000     Biso    1.000000 Ga
   Ga3     1.0     0.500000     0.000000     0.000000     Biso    1.000000 Ga
   Ga4     1.0     0.000000     0.500000     0.000000     Biso    1.000000 Ga
   Ga5     1.0     0.333333     0.666667     0.111111     Biso    1.000000 Ga
   Ga6     1.0     0.833333     0.666667     0.111111     Biso    1.000000 Ga
   Ga7     1.0     0.833333     0.166667     0.111111     Biso    1.000000 Ga
```

Ga8	1.0	0.333333	0.166667	0.111111	Biso	1.000000 Ga
Ga9	1.0	0.666690	0.333381	0.222341	Biso	1.000000 Ga
Ga10	1.0	0.166619	0.833309	0.222341	Biso	1.000000 Ga
Ga11	1.0	0.166667	0.333333	0.222225	Biso	1.000000 Ga
Ga12	1.0	0.666690	0.833309	0.222341	Biso	1.000000 Ga
Ga13	1.0	0.001916	0.003832	0.335512	Biso	1.000000 Ga
Ga14	1.0	0.496168	0.498084	0.335512	Biso	1.000000 Ga
Ga15	1.0	0.500000	0.000000	0.333641	Biso	1.000000 Ga
Ga16	1.0	0.001916	0.498084	0.335512	Biso	1.000000 Ga
Ga17	1.0	0.140020	0.820010	0.420726	Biso	1.000000 Ga
Ga18	1.0	0.679990	0.359980	0.420726	Biso	1.000000 Ga
Ga19	1.0	0.679990	0.820010	0.420726	Biso	1.000000 Ga
As1	1.0	0.000000	0.000000	0.083333	Biso	1.000000 As
As2	1.0	0.000000	0.500000	0.083333	Biso	1.000000 As
As3	1.0	0.500000	0.000000	0.083333	Biso	1.000000 As
As4	1.0	0.500000	0.500000	0.083333	Biso	1.000000 As
As5	1.0	0.333333	0.666667	0.194444	Biso	1.000000 As
As6	1.0	0.333333	0.166667	0.194444	Biso	1.000000 As
As7	1.0	0.833333	0.166667	0.194444	Biso	1.000000 As
As8	1.0	0.833333	0.666667	0.194444	Biso	1.000000 As
As9	1.0	0.667626	0.335251	0.305895	Biso	1.000000 As
As10	1.0	0.667626	0.832374	0.305895	Biso	1.000000 As
As11	1.0	0.166667	0.333333	0.305048	Biso	1.000000 As
As12	1.0	0.164749	0.832374	0.305895	Biso	1.000000 As
As13	1.0	0.023233	0.046466	0.420436	Biso	1.000000 As
As14	1.0	0.023233	0.476767	0.420436	Biso	1.000000 As
As15	1.0	0.500000	0.000000	0.419480	Biso	1.000000 As
As16	1.0	0.453534	0.476767	0.420436	Biso	1.000000 As
As17	1.0	0.166667	0.333333	0.972222	Biso	1.000000 As
As18	1.0	0.166667	0.833333	0.972222	Biso	1.000000 As
As19	1.0	0.666667	0.833333	0.972222	Biso	1.000000 As
As20	1.0	0.666667	0.333333	0.972222	Biso	1.000000 As
H.1	1.0	0.666667	0.333333	0.918783	Biso	1.000000 H.
H.2	1.0	0.166667	0.833333	0.918783	Biso	1.000000 H.
H.3	1.0	0.666667	0.833333	0.918783	Biso	1.000000 H.
H.4	1.0	0.166667	0.333333	0.918783	Biso	1.000000 H.

3-5. (111)A Ga-vacancy(2×2)-TW; Energy: –234.25739 eV (–8.6088010 Hartrees)

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_cell_length_c                         29.14671
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120

loop_
_space_group_symop_operation_xyz
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loop_
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   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
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_atom_site_type_symbol

Ga1	1.0	0.000000	0.000000	0.000000	Biso	1.000000 Ga
Ga2	1.0	0.500000	0.500000	0.000000	Biso	1.000000 Ga
Ga3	1.0	0.500000	0.000000	0.000000	Biso	1.000000 Ga
Ga4	1.0	0.000000	0.500000	0.000000	Biso	1.000000 Ga
Ga5	1.0	0.333333	0.666667	0.111111	Biso	1.000000 Ga
Ga6	1.0	0.833333	0.666667	0.111111	Biso	1.000000 Ga
Ga7	1.0	0.833333	0.166667	0.111111	Biso	1.000000 Ga
Ga8	1.0	0.333333	0.166667	0.111111	Biso	1.000000 Ga
Ga9	1.0	0.666667	0.333333	0.222028	Biso	1.000000 Ga
Ga10	1.0	0.166667	0.833333	0.222028	Biso	1.000000 Ga
Ga11	1.0	0.166667	0.333333	0.222028	Biso	1.000000 Ga
Ga12	1.0	0.666667	0.833333	0.222028	Biso	1.000000 Ga
Ga13	1.0	0.000082	0.000041	0.333829	Biso	1.000000 Ga
Ga14	1.0	0.499959	0.499918	0.333829	Biso	1.000000 Ga
Ga15	1.0	0.499959	0.000041	0.333829	Biso	1.000000 Ga
Ga16	1.0	0.000000	0.500000	0.333964	Biso	1.000000 Ga
Ga17	1.0	0.167026	0.332974	0.447299	Biso	1.000000 Ga
Ga18	1.0	0.167026	0.834052	0.447299	Biso	1.000000 Ga
Ga19	1.0	0.665948	0.332974	0.447299	Biso	1.000000 Ga
Ga20	1.0	0.666667	0.833333	0.444958	Biso	1.000000 Ga
Ga21	1.0	0.307116	0.653558	0.532949	Biso	1.000000 Ga
Ga22	1.0	0.846442	0.653558	0.532949	Biso	1.000000 Ga
Ga23	1.0	0.846442	0.192884	0.532949	Biso	1.000000 Ga
As1	1.0	0.000000	0.000000	0.083333	Biso	1.000000 As
As2	1.0	0.000000	0.500000	0.083333	Biso	1.000000 As
As3	1.0	0.500000	0.000000	0.083333	Biso	1.000000 As
As4	1.0	0.500000	0.500000	0.083333	Biso	1.000000 As
As5	1.0	0.333333	0.666667	0.194444	Biso	1.000000 As
As6	1.0	0.333333	0.166667	0.194444	Biso	1.000000 As
As7	1.0	0.833333	0.166667	0.194444	Biso	1.000000 As
As8	1.0	0.833333	0.666667	0.194444	Biso	1.000000 As
As9	1.0	0.666667	0.333333	0.305692	Biso	1.000000 As
As10	1.0	0.666667	0.833333	0.305692	Biso	1.000000 As
As11	1.0	0.166667	0.333333	0.305692	Biso	1.000000 As
As12	1.0	0.166667	0.833333	0.305692	Biso	1.000000 As
As13	1.0	0.000780	0.000390	0.417726	Biso	1.000000 As
As14	1.0	0.000000	0.500000	0.417979	Biso	1.000000 As
As15	1.0	0.499610	0.000390	0.417727	Biso	1.000000 As
As16	1.0	0.499610	0.499220	0.417727	Biso	1.000000 As
As17	1.0	0.621425	0.310713	0.531840	Biso	1.000000 As
As18	1.0	0.666667	0.833333	0.530054	Biso	1.000000 As
As19	1.0	0.189287	0.310713	0.531840	Biso	1.000000 As
As20	1.0	0.189287	0.878575	0.531840	Biso	1.000000 As
As21	1.0	0.166667	0.333333	0.972222	Biso	1.000000 As
As22	1.0	0.166667	0.833333	0.972222	Biso	1.000000 As
As23	1.0	0.666667	0.833333	0.972222	Biso	1.000000 As
As24	1.0	0.666667	0.333333	0.972222	Biso	1.000000 As
H.1	1.0	0.666667	0.333333	0.918783	Biso	1.000000 H.
H.2	1.0	0.166667	0.833333	0.918783	Biso	1.000000 H.
H.3	1.0	0.666667	0.833333	0.918783	Biso	1.000000 H.
H.4	1.0	0.166667	0.333333	0.918783	Biso	1.000000 H.

3-6. (111)A Ga-vacancy(2×2)-WZ; Energy: –234.12491 eV (–8.6039325 Hartrees)

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_cell_length_b	7.93273
_cell_length_c	29.14671
_cell_angle_alpha	90

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_cell_angle_beta                        90
_cell_angle_gamma                       120

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
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   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Ga1        1.0     0.000000     0.000000     0.000000    Biso    1.000000 Ga
   Ga2        1.0     0.500000     0.500000     0.000000    Biso    1.000000 Ga
   Ga3        1.0     0.500000     0.000000     0.000000    Biso    1.000000 Ga
   Ga4        1.0     0.000000     0.500000     0.000000    Biso    1.000000 Ga
   Ga5        1.0     0.333333     0.666667     0.111111    Biso    1.000000 Ga
   Ga6        1.0     0.833333     0.666667     0.111111    Biso    1.000000 Ga
   Ga7        1.0     0.833333     0.166667     0.111111    Biso    1.000000 Ga
   Ga8        1.0     0.333333     0.166667     0.111111    Biso    1.000000 Ga
   Ga9        1.0     0.666667     0.333333     0.222028    Biso    1.000000 Ga
   Ga10       1.0     0.166667     0.833333     0.222028    Biso    1.000000 Ga
   Ga11       1.0     0.166667     0.333333     0.222028    Biso    1.000000 Ga
   Ga12       1.0     0.666667     0.833333     0.222028    Biso    1.000000 Ga
   Ga13       1.0    -0.000243     0.000243     0.333765    Biso    1.000000 Ga
   Ga14       1.0     0.500000     0.500000     0.333796    Biso    1.000000 Ga
   Ga15       1.0     0.500485     0.000243     0.333765    Biso    1.000000 Ga
   Ga16       1.0    -0.000243     0.499515     0.333765    Biso    1.000000 Ga
   Ga17       1.0     0.170340     0.335170     0.447663    Biso    1.000000 Ga
   Ga18       1.0     0.166667     0.833333     0.445161    Biso    1.000000 Ga
   Ga19       1.0     0.664830     0.335170     0.447663    Biso    1.000000 Ga
   Ga20       1.0     0.664830     0.829660     0.447663    Biso    1.000000 Ga
   Ga21       1.0    -0.013221     0.013221     0.532494    Biso    1.000000 Ga
   Ga22       1.0    -0.013221     0.473559     0.532494    Biso    1.000000 Ga
   Ga23       1.0     0.526442     0.013221     0.532494    Biso    1.000000 Ga
   As1        1.0     0.000000     0.000000     0.083333    Biso    1.000000 As
   As2        1.0     0.000000     0.500000     0.083333    Biso    1.000000 As
   As3        1.0     0.500000     0.000000     0.083333    Biso    1.000000 As
   As4        1.0     0.500000     0.500000     0.083333    Biso    1.000000 As
   As5        1.0     0.333333     0.666667     0.194444    Biso    1.000000 As
   As6        1.0     0.333333     0.166667     0.194444    Biso    1.000000 As
   As7        1.0     0.833333     0.166667     0.194444    Biso    1.000000 As
   As8        1.0     0.833333     0.666667     0.194444    Biso    1.000000 As
   As9        1.0     0.666667     0.333333     0.305692    Biso    1.000000 As
   As10       1.0     0.666667     0.833333     0.305692    Biso    1.000000 As
   As11       1.0     0.166667     0.333333     0.305692    Biso    1.000000 As
   As12       1.0     0.166667     0.833333     0.305692    Biso    1.000000 As
   As13       1.0    -0.000933     0.000933     0.417862    Biso    1.000000 As
   As14       1.0    -0.000933     0.498134     0.417862    Biso    1.000000 As
   As15       1.0     0.501865     0.000933     0.417863    Biso    1.000000 As
   As16       1.0     0.500000     0.500000     0.417189    Biso    1.000000 As
   As17       1.0     0.643757     0.356242     0.532485    Biso    1.000000 As
   As18       1.0     0.643757     0.787515     0.532485    Biso    1.000000 As
   As19       1.0     0.212485     0.356243     0.532485    Biso    1.000000 As
   As20       1.0     0.166667     0.833333     0.530387    Biso    1.000000 As
   As21       1.0     0.166667     0.333333     0.972222    Biso    1.000000 As
   As22       1.0     0.166667     0.833333     0.972222    Biso    1.000000 As
   As23       1.0     0.666667     0.833333     0.972222    Biso    1.000000 As
   As24       1.0     0.666667     0.333333     0.972222    Biso    1.000000 As
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H.1	1.0	0.666667	0.333333	0.918783	Biso	1.000000 H.
H.2	1.0	0.166667	0.833333	0.918783	Biso	1.000000 H.
H.3	1.0	0.666667	0.833333	0.918783	Biso	1.000000 H.
H.4	1.0	0.166667	0.333333	0.918783	Biso	1.000000 H.

3-7. (111)B filled(√19×√19); Energy: –881.60096 eV (–32.398240 Hartrees)

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loop_
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   _atom_site_fract_z
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   Ga2     1.0     0.648857     0.472420     0.000859     Biso    1.000000 Ga
   Ga3     1.0     0.236698     0.400966     0.016701     Biso    1.000000 Ga
   Ga4     1.0     0.888624     0.026633     0.016844     Biso    1.000000 Ga
   Ga5     1.0     0.404879     0.439260     0.000825     Biso    1.000000 Ga
   Ga6     1.0     0.829938     0.266249     0.006150     Biso    1.000000 Ga
   Ga7     1.0     0.682420     0.194733     0.000707     Biso    1.000000 Ga
   Ga8     1.0     0.610102     0.678880     0.017101     Biso    1.000000 Ga
   Ga9     1.0     0.215237     0.616485     0.017856     Biso    1.000000 Ga
   Ga10    1.0     0.694423     0.005180     0.017760     Biso    1.000000 Ga
   Ga11    1.0     0.826217     0.484349     0.017910     Biso    1.000000 Ga
   Ga12    1.0     0.476138     0.219936     0.006277     Biso    1.000000 Ga
   Ga13    1.0     0.648161     0.807814     0.107269     Biso    1.000000 Ga
   Ga14    1.0     0.859973     0.118364     0.113181     Biso    1.000000 Ga
   Ga15    1.0     0.180384     0.599289     0.117055     Biso    1.000000 Ga
   Ga16    1.0     0.231434     0.164182     0.103573     Biso    1.000000 Ga
   Ga17    1.0     0.912104     0.701741     0.102975     Biso    1.000000 Ga
   Ga18    1.0     0.746260     0.970597     0.117211     Biso    1.000000 Ga
   Ga19    1.0     0.547477     0.650469     0.113451     Biso    1.000000 Ga
   Ga20    1.0     0.707132     0.382620     0.116396     Biso    1.000000 Ga
   Ga21    1.0     0.436354     0.497067     0.116269     Biso    1.000000 Ga
   Ga22    1.0     0.373818     0.920780     0.103642     Biso    1.000000 Ga
   Ga23    1.0     0.069931     0.437842     0.107209     Biso    1.000000 Ga
   Ga24    1.0     0.017813     0.860149     0.107154     Biso    1.000000 Ga
   Ga25    1.0     0.130498     0.021579     0.103582     Biso    1.000000 Ga
   Ga26    1.0     0.483854     0.066713     0.108946     Biso    1.000000 Ga
   Ga27    1.0     0.975613     0.273633     0.108937     Biso    1.000000 Ga
   Ga28    1.0     0.328018     0.337789     0.113228     Biso    1.000000 Ga
   Ga29    1.0     0.808972     0.536111     0.117594     Biso    1.000000 Ga
   Ga30    1.0     0.592557     0.226441     0.116333     Biso    1.000000 Ga
   Ga31    1.0     0.276693     0.765711     0.108990     Biso    1.000000 Ga
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Ga32	1.0	0.828362	0.399994	0.223258	Biso	1.000000 Ga
Ga33	1.0	0.985288	0.139333	0.221525	Biso	1.000000 Ga
Ga34	1.0	0.349279	0.191246	0.221551	Biso	1.000000 Ga
Ga35	1.0	0.140183	0.879811	0.221410	Biso	1.000000 Ga
Ga36	1.0	0.453746	0.352092	0.223077	Biso	1.000000 Ga
Ga37	1.0	0.610229	0.087429	0.223239	Biso	1.000000 Ga
Ga38	1.0	0.880703	0.980207	0.222398	Biso	1.000000 Ga
Ga39	1.0	0.245176	0.035611	0.220107	Biso	1.000000 Ga
Ga40	1.0	0.506151	0.930183	0.221476	Biso	1.000000 Ga
Ga41	1.0	0.772408	0.822819	0.221421	Biso	1.000000 Ga
Ga42	1.0	0.033674	0.720347	0.221466	Biso	1.000000 Ga
Ga43	1.0	0.190771	0.455061	0.222476	Biso	1.000000 Ga
Ga44	1.0	0.931285	0.561919	0.221475	Biso	1.000000 Ga
Ga45	1.0	0.089789	0.296112	0.221481	Biso	1.000000 Ga
Ga46	1.0	0.720118	0.243621	0.223097	Biso	1.000000 Ga
Ga47	1.0	0.562124	0.510303	0.223076	Biso	1.000000 Ga
Ga48	1.0	0.400875	0.775983	0.221536	Biso	1.000000 Ga
Ga49	1.0	0.297800	0.618138	0.223217	Biso	1.000000 Ga
Ga50	1.0	0.665127	0.670539	0.222503	Biso	1.000000 Ga
Ga51	1.0	0.000000	0.000000	0.333333	Biso	1.000000 Ga
Ga52	1.0	0.684211	0.526316	0.333333	Biso	1.000000 Ga
Ga53	1.0	0.368421	0.052632	0.333333	Biso	1.000000 Ga
Ga54	1.0	0.842105	0.263158	0.333333	Biso	1.000000 Ga
Ga55	1.0	0.526316	0.789474	0.333333	Biso	1.000000 Ga
Ga56	1.0	0.894737	0.842105	0.333333	Biso	1.000000 Ga
Ga57	1.0	0.052632	0.578947	0.333333	Biso	1.000000 Ga
Ga58	1.0	0.315789	0.473684	0.333333	Biso	1.000000 Ga
Ga59	1.0	0.210526	0.315789	0.333333	Biso	1.000000 Ga
Ga60	1.0	0.473684	0.210526	0.333333	Biso	1.000000 Ga
Ga61	1.0	0.631579	0.947368	0.333333	Biso	1.000000 Ga
Ga62	1.0	0.947368	0.421053	0.333333	Biso	1.000000 Ga
Ga63	1.0	0.789474	0.684210	0.333333	Biso	1.000000 Ga
Ga64	1.0	0.157895	0.736842	0.333333	Biso	1.000000 Ga
Ga65	1.0	0.736842	0.105263	0.333333	Biso	1.000000 Ga
Ga66	1.0	0.105263	0.157895	0.333333	Biso	1.000000 Ga
Ga67	1.0	0.263158	0.894737	0.333333	Biso	1.000000 Ga
Ga68	1.0	0.421053	0.631579	0.333333	Biso	1.000000 Ga
Ga69	1.0	0.578947	0.368421	0.333333	Biso	1.000000 Ga
Ga70	1.0	0.754386	0.964912	0.444444	Biso	1.000000 Ga
Ga71	1.0	0.701754	0.385965	0.444444	Biso	1.000000 Ga
Ga72	1.0	0.280702	0.754386	0.444444	Biso	1.000000 Ga
Ga73	1.0	0.859649	0.122807	0.444444	Biso	1.000000 Ga
Ga74	1.0	0.543860	0.649123	0.444444	Biso	1.000000 Ga
Ga75	1.0	0.438597	0.491228	0.444444	Biso	1.000000 Ga
Ga76	1.0	0.017544	0.859649	0.444444	Biso	1.000000 Ga
Ga77	1.0	0.122807	0.017544	0.444444	Biso	1.000000 Ga
Ga78	1.0	0.228070	0.175438	0.444444	Biso	1.000000 Ga
Ga79	1.0	0.385965	0.912281	0.444444	Biso	1.000000 Ga
Ga80	1.0	0.491228	0.070175	0.444444	Biso	1.000000 Ga
Ga81	1.0	0.175439	0.596491	0.444444	Biso	1.000000 Ga
Ga82	1.0	0.333333	0.333333	0.444444	Biso	1.000000 Ga
Ga83	1.0	0.649123	0.807017	0.444444	Biso	1.000000 Ga
Ga84	1.0	0.807018	0.543860	0.444444	Biso	1.000000 Ga
Ga85	1.0	0.964912	0.280702	0.444444	Biso	1.000000 Ga
Ga86	1.0	0.070176	0.438596	0.444444	Biso	1.000000 Ga
Ga87	1.0	0.912281	0.701754	0.444444	Biso	1.000000 Ga
Ga88	1.0	0.596492	0.228070	0.444444	Biso	1.000000 Ga
As1	1.0	0.607249	0.122679	0.963464	Biso	1.000000 As
As2	1.0	0.856121	0.904697	0.004212	Biso	1.000000 As
As3	1.0	0.578709	0.368787	0.012062	Biso	1.000000 As
As4	1.0	0.114561	0.555404	0.004096	Biso	1.000000 As
As5	1.0	0.764396	0.646118	0.004389	Biso	1.000000 As
As6	1.0	0.886142	0.852482	0.083201	Biso	1.000000 As

As7	1.0	0.370582	0.050837	0.069391	Biso	1.000000 As
As8	1.0	0.104728	0.160738	0.069296	Biso	1.000000 As
As9	1.0	0.210404	0.318176	0.077767	Biso	1.000000 As
As10	1.0	0.062648	0.576925	0.083195	Biso	1.000000 As
As11	1.0	0.631805	0.951900	0.079593	Biso	1.000000 As
As12	1.0	0.997417	0.000696	0.077894	Biso	1.000000 As
As13	1.0	0.421483	0.635784	0.088056	Biso	1.000000 As
As14	1.0	0.683753	0.519791	0.081480	Biso	1.000000 As
As15	1.0	0.578738	0.368749	0.094271	Biso	1.000000 As
As16	1.0	0.527699	0.787875	0.078059	Biso	1.000000 As
As17	1.0	0.845547	0.258796	0.087839	Biso	1.000000 As
As18	1.0	0.322283	0.474155	0.081338	Biso	1.000000 As
As19	1.0	0.729534	0.112512	0.081345	Biso	1.000000 As
As20	1.0	0.787187	0.675759	0.083438	Biso	1.000000 As
As21	1.0	0.162168	0.732500	0.079723	Biso	1.000000 As
As22	1.0	0.260662	0.894708	0.069319	Biso	1.000000 As
As23	1.0	0.941872	0.421723	0.079942	Biso	1.000000 As
As24	1.0	0.468665	0.211820	0.087905	Biso	1.000000 As
As25	1.0	0.860401	0.121528	0.195768	Biso	1.000000 As
As26	1.0	0.648165	0.809506	0.191840	Biso	1.000000 As
As27	1.0	0.177224	0.595296	0.198452	Biso	1.000000 As
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As29	1.0	0.753692	0.966756	0.198673	Biso	1.000000 As
As30	1.0	0.912478	0.701684	0.189396	Biso	1.000000 As
As31	1.0	0.543660	0.651039	0.196090	Biso	1.000000 As
As32	1.0	0.019838	0.857933	0.191763	Biso	1.000000 As
As33	1.0	0.385617	0.912791	0.189659	Biso	1.000000 As
As34	1.0	0.068845	0.437887	0.191832	Biso	1.000000 As
As35	1.0	0.703025	0.384930	0.198295	Biso	1.000000 As
As36	1.0	0.122288	0.018108	0.189636	Biso	1.000000 As
As37	1.0	0.438067	0.493014	0.198138	Biso	1.000000 As
As38	1.0	0.490002	0.069402	0.193002	Biso	1.000000 As
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As40	1.0	0.331613	0.333826	0.195852	Biso	1.000000 As
As41	1.0	0.595007	0.227799	0.198238	Biso	1.000000 As
As42	1.0	0.279384	0.756525	0.192938	Biso	1.000000 As
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As45	1.0	0.982456	0.140351	0.305555	Biso	1.000000 As
As46	1.0	0.877193	0.982456	0.305555	Biso	1.000000 As
As47	1.0	0.140351	0.877193	0.305555	Biso	1.000000 As
As48	1.0	0.298246	0.614035	0.305555	Biso	1.000000 As
As49	1.0	0.561404	0.508772	0.305555	Biso	1.000000 As
As50	1.0	0.666667	0.666667	0.305555	Biso	1.000000 As
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As53	1.0	0.719298	0.245614	0.305555	Biso	1.000000 As
As54	1.0	0.614035	0.087719	0.305555	Biso	1.000000 As
As55	1.0	0.456140	0.350877	0.305555	Biso	1.000000 As
As56	1.0	0.035088	0.719298	0.305555	Biso	1.000000 As
As57	1.0	0.350877	0.192982	0.305555	Biso	1.000000 As
As58	1.0	0.508772	0.929824	0.305555	Biso	1.000000 As
As59	1.0	0.245614	0.035088	0.305555	Biso	1.000000 As
As60	1.0	0.087719	0.298246	0.305555	Biso	1.000000 As
As61	1.0	0.192982	0.456140	0.305555	Biso	1.000000 As
As62	1.0	0.403509	0.771930	0.305555	Biso	1.000000 As
As63	1.0	0.210526	0.315789	0.416667	Biso	1.000000 As
As64	1.0	0.052632	0.578947	0.416667	Biso	1.000000 As
As65	1.0	0.736842	0.105263	0.416667	Biso	1.000000 As
As66	1.0	0.105263	0.157895	0.416667	Biso	1.000000 As
As67	1.0	0.947368	0.421053	0.416667	Biso	1.000000 As
As68	1.0	0.842105	0.263158	0.416667	Biso	1.000000 As
As69	1.0	0.684211	0.526316	0.416667	Biso	1.000000 As

As70	1.0	0.526316	0.789474	0.416667	Biso	1.000000 As
As71	1.0	0.578947	0.368421	0.416667	Biso	1.000000 As
As72	1.0	0.421053	0.631579	0.416667	Biso	1.000000 As
As73	1.0	0.315789	0.473684	0.416667	Biso	1.000000 As
As74	1.0	0.263158	0.894737	0.416667	Biso	1.000000 As
As75	1.0	0.894737	0.842105	0.416667	Biso	1.000000 As
As76	1.0	0.789474	0.684210	0.416667	Biso	1.000000 As
As77	1.0	0.000000	0.000000	0.416667	Biso	1.000000 As
As78	1.0	0.368421	0.052632	0.416667	Biso	1.000000 As
As79	1.0	0.631579	0.947368	0.416667	Biso	1.000000 As
As80	1.0	0.473684	0.210526	0.416667	Biso	1.000000 As
As81	1.0	0.157895	0.736842	0.416667	Biso	1.000000 As
As82	1.0	0.825841	0.150166	0.963292	Biso	1.000000 As
As83	1.0	0.549699	0.615774	0.963691	Biso	1.000000 As
As84	1.0	0.332637	0.586409	0.963535	Biso	1.000000 As
As85	1.0	0.795744	0.397701	0.963370	Biso	1.000000 As
As86	1.0	0.360622	0.340351	0.963307	Biso	1.000000 As
H11	1.0	0.017544	0.859649	0.497912	Biso	1.000000 H1
H12	1.0	0.754386	0.964912	0.497912	Biso	1.000000 H1
H13	1.0	0.596492	0.228070	0.497912	Biso	1.000000 H1
H14	1.0	0.543860	0.649123	0.497912	Biso	1.000000 H1
H15	1.0	0.859649	0.122807	0.497912	Biso	1.000000 H1
H16	1.0	0.912281	0.701754	0.497912	Biso	1.000000 H1
H17	1.0	0.070176	0.438596	0.497912	Biso	1.000000 H1
H18	1.0	0.385965	0.912281	0.497912	Biso	1.000000 H1
H19	1.0	0.228070	0.175438	0.497912	Biso	1.000000 H1
H110	1.0	0.333333	0.333333	0.497912	Biso	1.000000 H1
H111	1.0	0.807018	0.543860	0.497912	Biso	1.000000 H1
H112	1.0	0.964912	0.280702	0.497912	Biso	1.000000 H1
H113	1.0	0.122807	0.017544	0.497912	Biso	1.000000 H1
H114	1.0	0.649123	0.807017	0.497912	Biso	1.000000 H1
H115	1.0	0.491228	0.070175	0.497912	Biso	1.000000 H1
H116	1.0	0.175439	0.596491	0.497912	Biso	1.000000 H1
H117	1.0	0.280702	0.754386	0.497912	Biso	1.000000 H1
H118	1.0	0.438597	0.491228	0.497912	Biso	1.000000 H1
H119	1.0	0.701754	0.385965	0.497912	Biso	1.000000 H1

3-8. (111)B Ga-vacancy α(2×2)-ZB; Energy: –188.56369 eV (–6.9295884 Hartrees)

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Ga3	1.0	0.696309	0.392619	0.993775	Biso	1.000000 Ga
Ga4	1.0	0.050423	0.100846	0.996101	Biso	1.000000 Ga
Ga5	1.0	0.399154	0.449577	0.996101	Biso	1.000000 Ga
Ga6	1.0	0.500000	0.000000	0.995108	Biso	1.000000 Ga
Ga7	1.0	0.050423	0.449577	0.996101	Biso	1.000000 Ga
Ga8	1.0	0.333903	0.667806	0.111436	Biso	1.000000 Ga
Ga9	1.0	0.833333	0.666667	0.109675	Biso	1.000000 Ga
Ga10	1.0	0.832194	0.166097	0.111436	Biso	1.000000 Ga
Ga11	1.0	0.333903	0.166097	0.111436	Biso	1.000000 Ga
Ga12	1.0	0.666667	0.333333	0.222222	Biso	1.000000 Ga
Ga13	1.0	0.166667	0.833333	0.222222	Biso	1.000000 Ga
Ga14	1.0	0.166667	0.333333	0.222222	Biso	1.000000 Ga
Ga15	1.0	0.666667	0.833333	0.222222	Biso	1.000000 Ga
Ga16	1.0	0.000000	0.000000	0.333333	Biso	1.000000 Ga
Ga17	1.0	0.500000	0.500000	0.333333	Biso	1.000000 Ga
Ga18	1.0	0.500000	0.000000	0.333333	Biso	1.000000 Ga
Ga19	1.0	0.000000	0.500000	0.333333	Biso	1.000000 Ga
Ga20	1.0	0.333333	0.666667	0.444444	Biso	1.000000 Ga
Ga21	1.0	0.833333	0.666667	0.444444	Biso	1.000000 Ga
Ga22	1.0	0.833333	0.166667	0.444444	Biso	1.000000 Ga
Ga23	1.0	0.333333	0.166667	0.444444	Biso	1.000000 Ga
As1	1.0	0.000903	0.001806	0.080366	Biso	1.000000 As
As2	1.0	0.000903	0.499097	0.080366	Biso	1.000000 As
As3	1.0	0.500000	0.000000	0.080861	Biso	1.000000 As
As4	1.0	0.498194	0.499097	0.080366	Biso	1.000000 As
As5	1.0	0.333333	0.666666	0.194677	Biso	1.000000 As
As6	1.0	0.333333	0.166667	0.194677	Biso	1.000000 As
As7	1.0	0.833334	0.166667	0.194677	Biso	1.000000 As
As8	1.0	0.833333	0.666667	0.193436	Biso	1.000000 As
As9	1.0	0.666667	0.333333	0.305555	Biso	1.000000 As
As10	1.0	0.666667	0.833333	0.305555	Biso	1.000000 As
As11	1.0	0.166667	0.333333	0.305555	Biso	1.000000 As
As12	1.0	0.166667	0.833333	0.305555	Biso	1.000000 As
As13	1.0	0.000000	0.000000	0.416667	Biso	1.000000 As
As14	1.0	0.000000	0.500000	0.416667	Biso	1.000000 As
As15	1.0	0.500000	0.000000	0.416667	Biso	1.000000 As
As16	1.0	0.500000	0.500000	0.416667	Biso	1.000000 As
H11	1.0	0.333333	0.666667	0.497912	Biso	1.000000 H1
H12	1.0	0.333333	0.166667	0.497912	Biso	1.000000 H1
H13	1.0	0.833333	0.666667	0.497912	Biso	1.000000 H1
H14	1.0	0.833333	0.166667	0.497912	Biso	1.000000 H1

3-9. (111)B Ga-vacancy α(2×2)-SF; Energy: –188.42184 eV (–6.9243755 Hartrees)

```
_chemical_name_common                  '111B Ga-vacancy a-SF'
_cell_length_a                         7.93273
_cell_length_b                         7.93273
_cell_length_c                         29.14671
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120

loop_
_space_group_symop_operation_xyz
   'x, y, z'
```

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loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Ga1     1.0     0.399157     0.699579     0.991879     Biso    1.000000 Ga
   Ga2     1.0     0.800421     0.100843     0.991879     Biso    1.000000 Ga
   Ga3     1.0     0.800421     0.699579     0.991879     Biso    1.000000 Ga
   Ga4     1.0     0.101704     0.050852     0.995469     Biso    1.000000 Ga
   Ga5     1.0     0.449148     0.398296     0.995469     Biso    1.000000 Ga
   Ga6     1.0     0.449148     0.050852     0.995469     Biso    1.000000 Ga
   Ga7     1.0     0.000000     0.500000     0.994139     Biso    1.000000 Ga
   Ga8     1.0     0.331523     0.665761     0.110600     Biso    1.000000 Ga
   Ga9     1.0     0.834239     0.665761     0.110600     Biso    1.000000 Ga
   Ga10    1.0     0.834239     0.168477     0.110600     Biso    1.000000 Ga
   Ga11    1.0     0.333333     0.166667     0.112033     Biso    1.000000 Ga
   Ga12    1.0     0.666667     0.333333     0.222222     Biso    1.000000 Ga
   Ga13    1.0     0.166667     0.833333     0.222222     Biso    1.000000 Ga
   Ga14    1.0     0.166667     0.333333     0.222222     Biso    1.000000 Ga
   Ga15    1.0     0.666667     0.833333     0.222222     Biso    1.000000 Ga
   Ga16    1.0     0.000000     0.000000     0.333333     Biso    1.000000 Ga
   Ga17    1.0     0.500000     0.500000     0.333333     Biso    1.000000 Ga
   Ga18    1.0     0.500000     0.000000     0.333333     Biso    1.000000 Ga
   Ga19    1.0     0.000000     0.500000     0.333333     Biso    1.000000 Ga
   Ga20    1.0     0.333333     0.666667     0.444444     Biso    1.000000 Ga
   Ga21    1.0     0.833333     0.666667     0.444444     Biso    1.000000 Ga
   Ga22    1.0     0.833333     0.166667     0.444444     Biso    1.000000 Ga
   Ga23    1.0     0.333333     0.166667     0.444444     Biso    1.000000 Ga
   As1     1.0     0.000750     0.000375     0.080264     Biso    1.000000 As
   As2     1.0     0.000000     0.500000     0.080326     Biso    1.000000 As
   As3     1.0     0.499625     0.000375     0.080264     Biso    1.000000 As
   As4     1.0     0.499625     0.499249     0.080264     Biso    1.000000 As
   As5     1.0     0.333849     0.666925     0.194243     Biso    1.000000 As
   As6     1.0     0.333333     0.166667     0.194930     Biso    1.000000 As
   As7     1.0     0.833075     0.166151     0.194243     Biso    1.000000 As
   As8     1.0     0.833075     0.666925     0.194243     Biso    1.000000 As
   As9     1.0     0.666667     0.333333     0.305555     Biso    1.000000 As
   As10    1.0     0.666667     0.833333     0.305555     Biso    1.000000 As
   As11    1.0     0.166667     0.333333     0.305555     Biso    1.000000 As
   As12    1.0     0.166667     0.833333     0.305555     Biso    1.000000 As
   As13    1.0     0.000000     0.000000     0.416667     Biso    1.000000 As
   As14    1.0     0.000000     0.500000     0.416667     Biso    1.000000 As
   As15    1.0     0.500000     0.000000     0.416667     Biso    1.000000 As
   As16    1.0     0.500000     0.500000     0.416667     Biso    1.000000 As
   H11     1.0     0.333333     0.666667     0.497912     Biso    1.000000 H1
   H12     1.0     0.333333     0.166667     0.497912     Biso    1.000000 H1
   H13     1.0     0.833333     0.666667     0.497912     Biso    1.000000 H1
   H14     1.0     0.833333     0.166667     0.497912     Biso    1.000000 H1
```

3-10. (111)B Ga-vacancy α(2×2)-TW; Energy: –226.91858 eV (–8.3391047 Hartrees)

```
_chemical_name_common                  '111B Ga-vacancy a-TW '
_cell_length_a                         7.93273
_cell_length_b                         7.93273
_cell_length_c                         29.14671
```

```
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                        120

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Ga1        1.0     0.726059     0.363030     0.881456    Biso   1.000000 Ga
   Ga2        1.0     0.136970     0.773941     0.881456    Biso   1.000000 Ga
   Ga3        1.0     0.136970     0.363030     0.881456    Biso   1.000000 Ga
   Ga4        1.0     0.434356     0.717178     0.883665    Biso   1.000000 Ga
   Ga5        1.0     0.782822     0.717178     0.883665    Biso   1.000000 Ga
   Ga6        1.0     0.782822     0.065644     0.883665    Biso   1.000000 Ga
   Ga7        1.0     0.333333     0.166667     0.883846    Biso   1.000000 Ga
   Ga8        1.0    -0.000081    -0.000041    -0.000696    Biso   1.000000 Ga
   Ga9        1.0     0.500041     0.500081    -0.000696    Biso   1.000000 Ga
   Ga10       1.0     0.500040    -0.000041    -0.000696    Biso   1.000000 Ga
   Ga11       1.0     0.000000     0.500000    -0.002192    Biso   1.000000 Ga
   Ga12       1.0     0.333333     0.666667     0.110814    Biso   1.000000 Ga
   Ga13       1.0     0.833333     0.666667     0.110814    Biso   1.000000 Ga
   Ga14       1.0     0.833333     0.166667     0.110814    Biso   1.000000 Ga
   Ga15       1.0     0.333333     0.166667     0.110814    Biso   1.000000 Ga
   Ga16       1.0     0.666667     0.333333     0.222222    Biso   1.000000 Ga
   Ga17       1.0     0.166667     0.833333     0.222222    Biso   1.000000 Ga
   Ga18       1.0     0.166667     0.333333     0.222222    Biso   1.000000 Ga
   Ga19       1.0     0.666667     0.833333     0.222222    Biso   1.000000 Ga
   Ga20       1.0     0.000000     0.000000     0.333333    Biso   1.000000 Ga
   Ga21       1.0     0.500000     0.500000     0.333333    Biso   1.000000 Ga
   Ga22       1.0     0.500000     0.000000     0.333333    Biso   1.000000 Ga
   Ga23       1.0     0.000000     0.500000     0.333333    Biso   1.000000 Ga
   Ga24       1.0     0.333333     0.666667     0.444444    Biso   1.000000 Ga
   Ga25       1.0     0.833333     0.666667     0.444444    Biso   1.000000 Ga
   Ga26       1.0     0.833333     0.166667     0.444444    Biso   1.000000 Ga
   Ga27       1.0     0.333333     0.166667     0.444444    Biso   1.000000 Ga
   As1        1.0     0.333333     0.166667     0.969532    Biso   1.000000 As
   As2        1.0     0.334693     0.667346     0.967874    Biso   1.000000 As
   As3        1.0     0.832654     0.165307     0.967874    Biso   1.000000 As
   As4        1.0     0.832654     0.667346     0.967874    Biso   1.000000 As
   As5        1.0    -0.000171    -0.000086     0.082877    Biso   1.000000 As
   As6        1.0     0.000000     0.500000     0.082180    Biso   1.000000 As
   As7        1.0     0.500086    -0.000086     0.082877    Biso   1.000000 As
   As8        1.0     0.500086     0.500171     0.082877    Biso   1.000000 As
   As9        1.0     0.333333     0.666667     0.194663    Biso   1.000000 As
   As10       1.0     0.333333     0.166667     0.194663    Biso   1.000000 As
   As11       1.0     0.833333     0.166667     0.194663    Biso   1.000000 As
   As12       1.0     0.833333     0.666667     0.194663    Biso   1.000000 As
   As13       1.0     0.666667     0.333333     0.305555    Biso   1.000000 As
   As14       1.0     0.666667     0.833333     0.305555    Biso   1.000000 As
   As15       1.0     0.166667     0.333333     0.305555    Biso   1.000000 As
   As16       1.0     0.166667     0.833333     0.305555    Biso   1.000000 As
   As17       1.0     0.000000     0.000000     0.416667    Biso   1.000000 As
   As18       1.0     0.000000     0.500000     0.416667    Biso   1.000000 As
   As19       1.0     0.500000     0.000000     0.416667    Biso   1.000000 As
```

As20	1.0	0.500000	0.500000	0.416667	Biso	1.000000 As
H11	1.0	0.333333	0.666667	0.497912	Biso	1.000000 H1
H12	1.0	0.333333	0.166667	0.497912	Biso	1.000000 H1
H13	1.0	0.833333	0.666667	0.497912	Biso	1.000000 H1
H14	1.0	0.833333	0.166667	0.497912	Biso	1.000000 H1

3-11. (111)B Ga-vacancy α(2×2)-WZ; Energy: –226.81280 eV (–8.3352174 Hartrees)

```
_chemical_name_common                  '111B Ga-vacancy a-WZ'
_cell_length_a                         7.93273
_cell_length_b                         7.93273
_cell_length_c                         29.14671
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                        120

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Ga1          1.0     0.032283     -0.032283     0.880257     Biso   1.000000 Ga
   Ga2          1.0     0.032283     0.564565      0.880257     Biso   1.000000 Ga
   Ga3          1.0     0.435435     -0.032283     0.880257     Biso   1.000000 Ga
   Ga4          1.0     0.384220     0.615779      0.883420     Biso   1.000000 Ga
   Ga5          1.0     0.731559     0.615779      0.883420     Biso   1.000000 Ga
   Ga6          1.0     0.833333     0.166667      0.881861     Biso   1.000000 Ga
   Ga7          1.0     0.384220     0.268441      0.883420     Biso   1.000000 Ga
   Ga8          1.0     -0.000956    0.000956      -0.001503    Biso   1.000000 Ga
   Ga9          1.0     0.500000     0.500000      0.000031     Biso   1.000000 Ga
   Ga10         1.0     0.501913     0.000956      -0.001503    Biso   1.000000 Ga
   Ga11         1.0     -0.000956    0.498087      -0.001503    Biso   1.000000 Ga
   Ga12         1.0     0.333333     0.666667      0.110814     Biso   1.000000 Ga
   Ga13         1.0     0.833333     0.666667      0.110814     Biso   1.000000 Ga
   Ga14         1.0     0.833333     0.166667      0.110814     Biso   1.000000 Ga
   Ga15         1.0     0.333333     0.166667      0.110814     Biso   1.000000 Ga
   Ga16         1.0     0.666667     0.333333      0.222222     Biso   1.000000 Ga
   Ga17         1.0     0.166667     0.833333      0.222222     Biso   1.000000 Ga
   Ga18         1.0     0.166667     0.333333      0.222222     Biso   1.000000 Ga
   Ga19         1.0     0.666667     0.833333      0.222222     Biso   1.000000 Ga
   Ga20         1.0     0.000000     0.000000      0.333333     Biso   1.000000 Ga
   Ga21         1.0     0.500000     0.500000      0.333333     Biso   1.000000 Ga
   Ga22         1.0     0.500000     0.000000      0.333333     Biso   1.000000 Ga
   Ga23         1.0     0.000000     0.500000      0.333333     Biso   1.000000 Ga
   Ga24         1.0     0.333333     0.666667      0.444444     Biso   1.000000 Ga
   Ga25         1.0     0.833333     0.666667      0.444444     Biso   1.000000 Ga
   Ga26         1.0     0.833333     0.166667      0.444444     Biso   1.000000 Ga
   Ga27         1.0     0.333333     0.166667      0.444444     Biso   1.000000 Ga
   As1          1.0     0.333644     0.167289      0.967869     Biso   1.000000 As
   As2          1.0     0.333644     0.666356      0.967869     Biso   1.000000 As
   As3          1.0     0.833333     0.166667      0.967834     Biso   1.000000 As
```

As4	1.0	0.832711	0.666356	0.967868	Biso	1.000000 As
As5	1.0	0.000049	−0.000049	0.082489	Biso	1.000000 As
As6	1.0	0.000049	0.500097	0.082489	Biso	1.000000 As
As7	1.0	0.499903	−0.000049	0.082489	Biso	1.000000 As
As8	1.0	0.500000	0.500000	0.083343	Biso	1.000000 As
As9	1.0	0.333333	0.666667	0.194663	Biso	1.000000 As
As10	1.0	0.333333	0.166667	0.194663	Biso	1.000000 As
As11	1.0	0.833333	0.166667	0.194663	Biso	1.000000 As
As12	1.0	0.833333	0.666667	0.194663	Biso	1.000000 As
As13	1.0	0.666667	0.333333	0.305555	Biso	1.000000 As
As14	1.0	0.666667	0.833333	0.305555	Biso	1.000000 As
As15	1.0	0.166667	0.333333	0.305555	Biso	1.000000 As
As16	1.0	0.166667	0.833333	0.305555	Biso	1.000000 As
As17	1.0	0.000000	0.000000	0.416667	Biso	1.000000 As
As18	1.0	0.000000	0.500000	0.416667	Biso	1.000000 As
As19	1.0	0.500000	0.000000	0.416667	Biso	1.000000 As
As20	1.0	0.500000	0.500000	0.416667	Biso	1.000000 As
H11	1.0	0.333333	0.666667	0.497912	Biso	1.000000 H1
H12	1.0	0.333333	0.166667	0.497912	Biso	1.000000 H1
H13	1.0	0.833333	0.666667	0.497912	Biso	1.000000 H1
H14	1.0	0.833333	0.166667	0.497912	Biso	1.000000 H1