Tuning Energy Band-gap of Gallium Oxide Crystalline to Enhance Photoelectrochemical Water Splitting: Mixed-phase Junctions

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TABLE I: The calculated lattice constants of $\alpha$-Ga$_2$O$_3$ and $\beta$-Ga$_2$O$_3$ with the energy cutoff of 520 eV.

<table>
<thead>
<tr>
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<th>$\alpha$-Ga$_2$O$_3$</th>
<th>$\beta$-Ga$_2$O$_3$</th>
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<tbody>
<tr>
<td>$a$(Å)</td>
<td>5.05</td>
<td>12.44</td>
</tr>
<tr>
<td>$b$(Å)</td>
<td>3.08</td>
<td></td>
</tr>
<tr>
<td>$c$(Å)</td>
<td>13.63</td>
<td>5.87</td>
</tr>
<tr>
<td>$\gamma$(degree)</td>
<td>103.8</td>
<td></td>
</tr>
</tbody>
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Fig. 1: The total DOS of $\alpha$-Ga$_2$O$_3$ and $\beta$-Ga$_2$O$_3$ by PBE.
Fig. 2: The total and projected DOS of per formula unit of α–Ga₂O₃ and β–Ga₂O₃ calculated by HSE06 functional. The conduction band are zoom in. The Fermi level is set to zero.

Fig. 3: The differences of PAC for the heterostructures (b-type) with the crystal axis angle(101°).
Fig. 4: The total DOS of periodic slab model of the heterostructures (α) with the different crystal axis angles 95° (left) and 101° (right).

Fig. 5: The LDOS of periodic slab model of the heterostructures (α) with the different crystal axis angles 95°, (left) and 101° (right).
Fig. 6: The optical absorption curves of the mixed-phase and the two pure phases by PBE.

Fig. 7: The calculated energies of $b$-type heterostructures A1-B1 with different lengths and the most stable heterostructure with length 45.8 Å. ($\phi = 101^\circ$)

Fig. 8: The total DOS of $b$-type heterostructures A1-B1 with length 45.8 Å. ($\phi = 101^\circ$)
Fig. 9: The LDOSs of $b$-type heterostructures A1-B1 with length 45.8 Å ($\phi = 101^\circ$)
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