

## Supplemental Material

### The electronic structures of $\beta$ -phase $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ studied by DFT calculations

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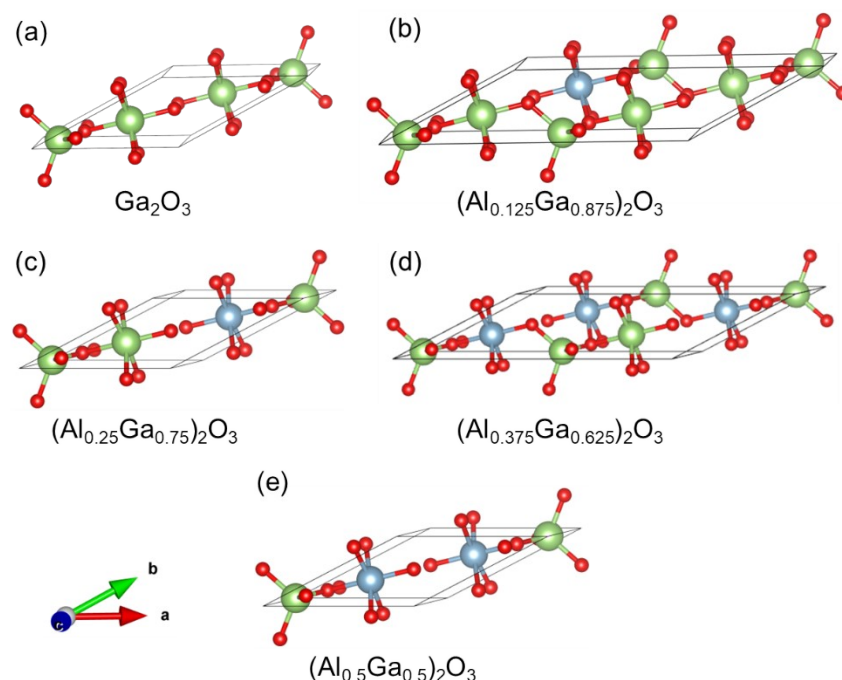
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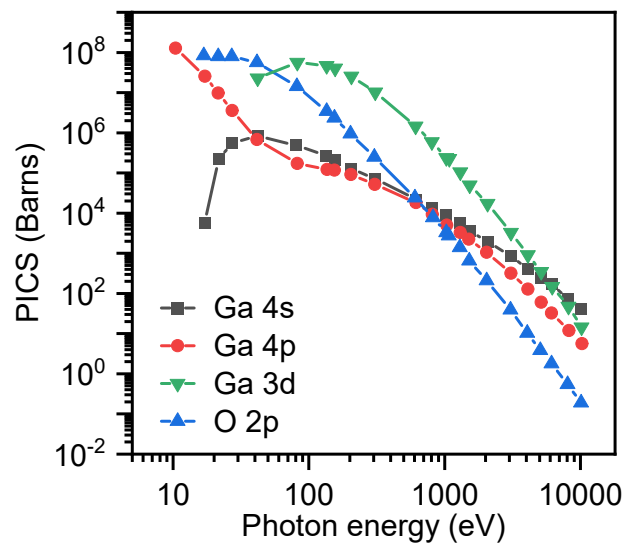
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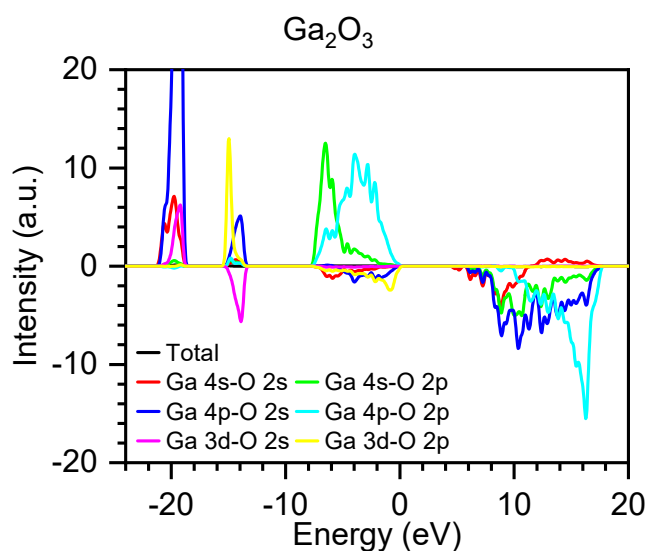
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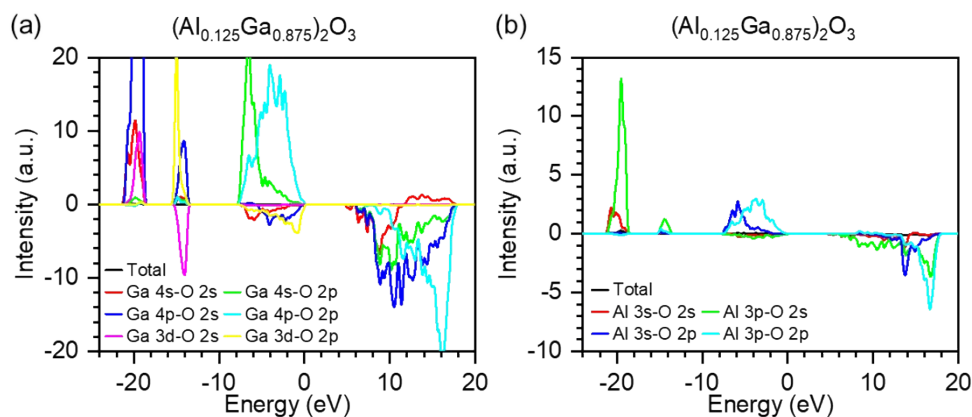
**Figure S1.** The crystal structure (a)  $\text{Ga}_2\text{O}_3$  primitive cell; (b)-(e)  $\beta$ - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloys for  $x = 0.125, 0.25, 0.375$  and  $0.50$ .



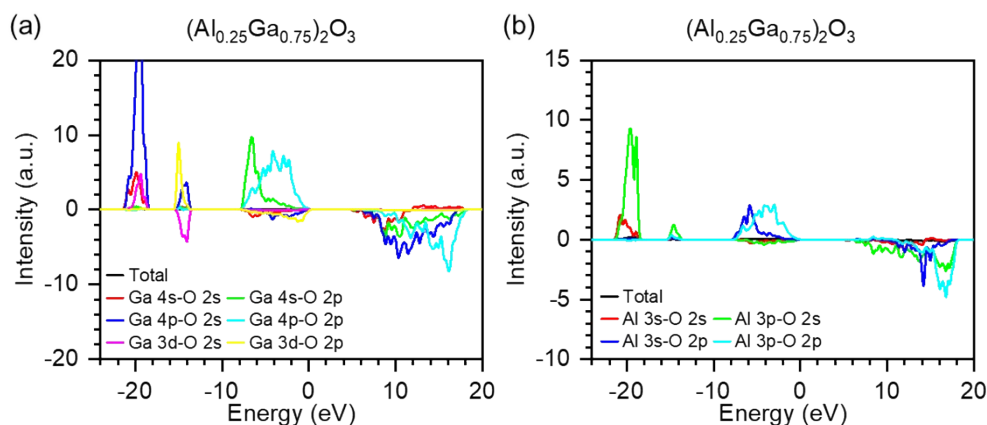
**Figure S2.** Relationship between the photoionization cross section of an electron and the photon energy of Ga 4s, Ga 4p, Ga 3d and O 2p.



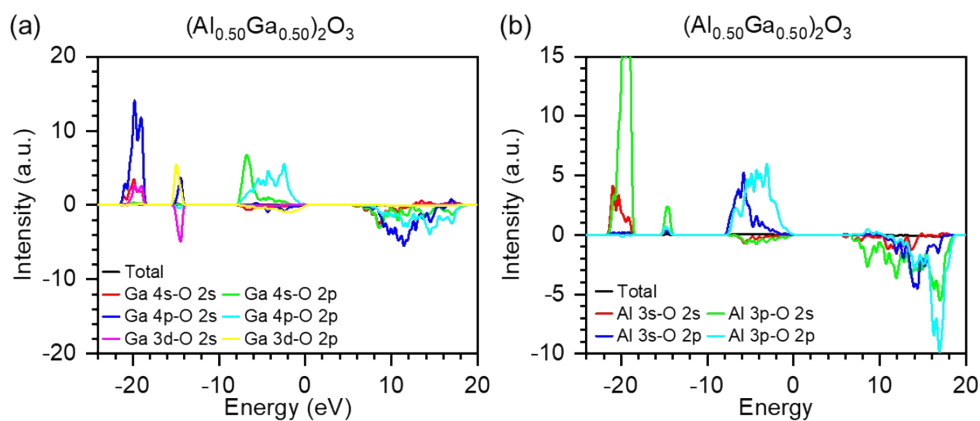
**Figure S3.** -pCOHP intensity of the orbital interactions between Ga and O atoms in  $\text{Ga}_2\text{O}_3$  and  $\beta\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloys of  $x = 0.125, 0.25$ , and  $0.50$ .



**Figure S4.** -pCOHP intensity of the orbital interactions between (a) Ga and O atoms (b) Al and O atoms for  $(\text{Al}_{0.125}\text{Ga}_{0.875})_2\text{O}_3$ .



**Figure S5.** -pCOHP intensity of the orbital interactions between (a) Ga and O atoms (b) Al and O atoms for  $(\text{Al}_{0.25}\text{Ga}_{0.75})_2\text{O}_3$ .



**Figure S6.** -pCOHP intensity of the orbital interactions between (a) Ga and O atoms (b) Al and O atoms for  $(\text{Al}_{0.50}\text{Ga}_{0.50})_2\text{O}_3$ .