

Supplemental Material

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

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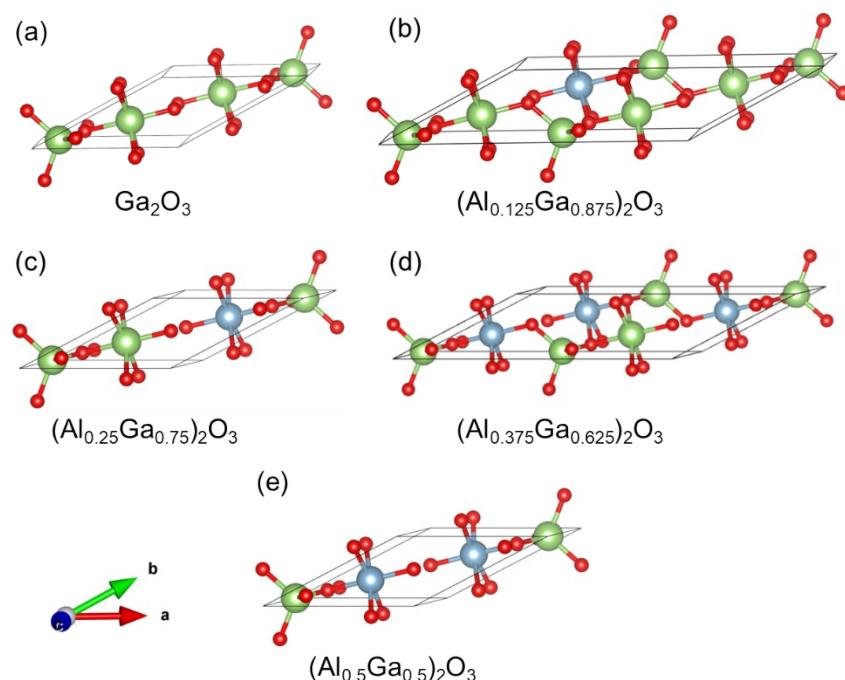


Figure S1. The crystal structure (a) Ga_2O_3 primitive cell; (b)-(e) β - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ alloys for $x = 0.125, 0.25, 0.375$ and 0.50 .

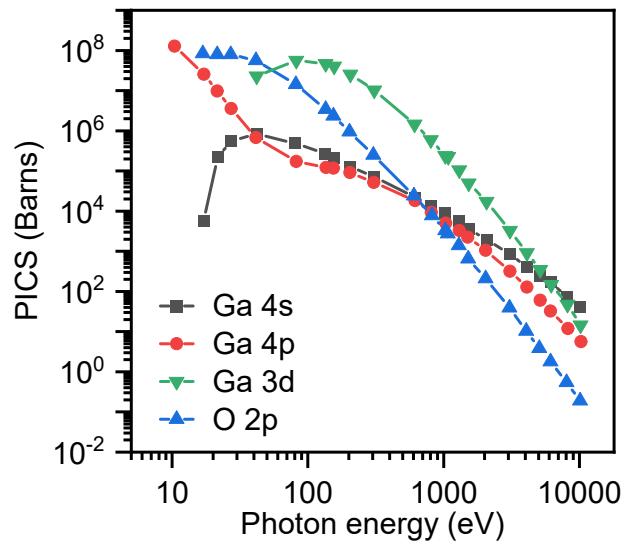


Figure S2. Relationship between the photoionization cross section of an electron and the photon energy of Ga 4s, Ga 4p, Ga 3d and O 2p.

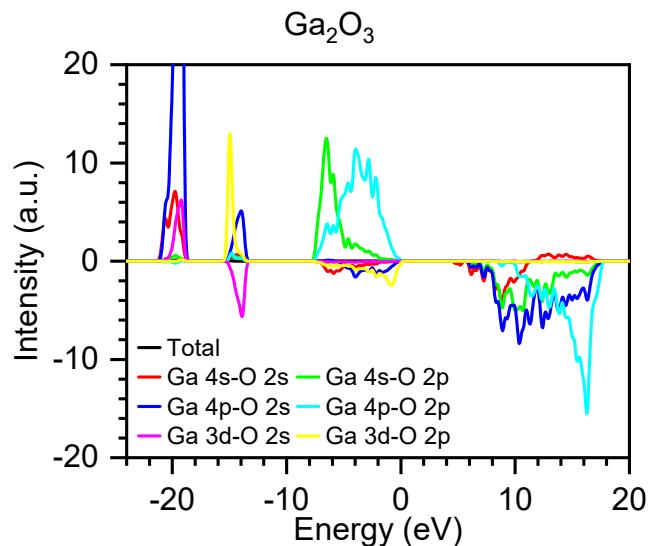


Figure S3. -pCOHP intensity of the orbital interactions between Ga and O atoms in Ga_2O_3 and $\beta-(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ alloys of $x = 0.125, 0.25$, and 0.50 .

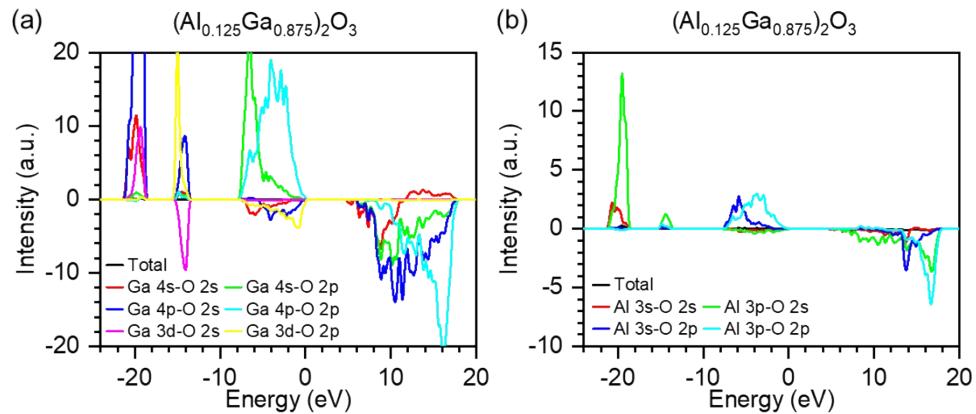


Figure S4. -pCOHP intensity of the orbital interactions between (a) Ga and O atoms (b) Al and O atoms for $(Al_{0.125}Ga_{0.875})_2O_3$.

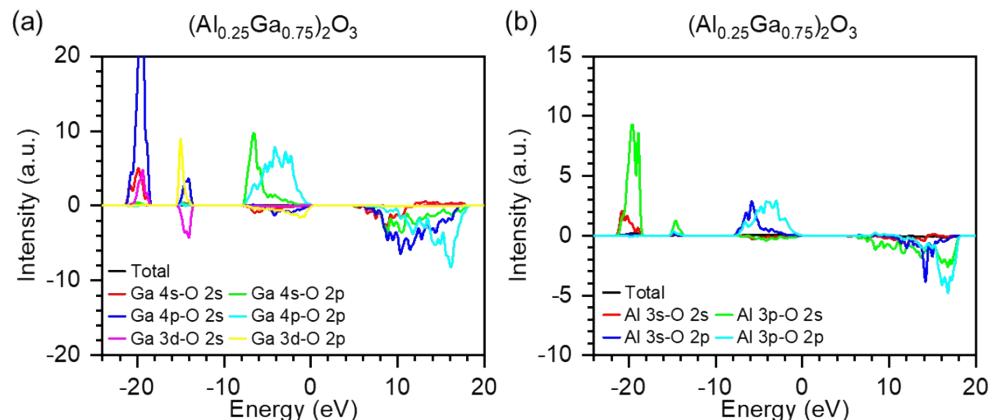


Figure S5. -pCOHP intensity of the orbital interactions between (a) Ga and O atoms (b) Al and O atoms for $(Al_{0.25}Ga_{0.75})_2O_3$.

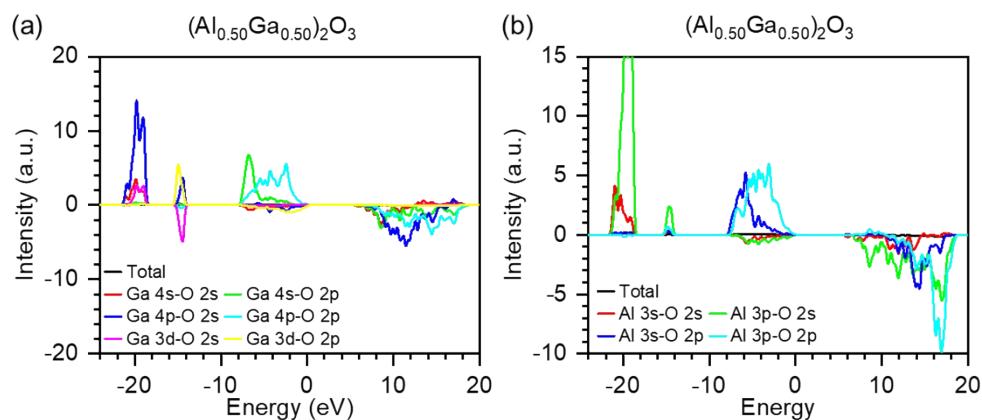


Figure S6. -pCOHP intensity of the orbital interactions between (a) Ga and O atoms (b) Al and O atoms for $(Al_{0.50}Ga_{0.50})_2O_3$.