Supporting Information

First-principle study of Ga-vacancy induced magnetism in β-Ga_2O_3

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Table-S1. The structure information of relaxed β-Ga_2O_3:

Atom	x	y	z
Ga^{tetra}	0.09146	0	0.80094
Ga^{octa}	0.16217	0.50000	0.55585
O1	0.17776	0	0.11232
O2	0.16870	0	0.55585
O3	0.99952	0.50000	0.24872

C2/m, a = 12.214 Å, b = 3.037 Å, c = 5.798 Å and β = 103.830°

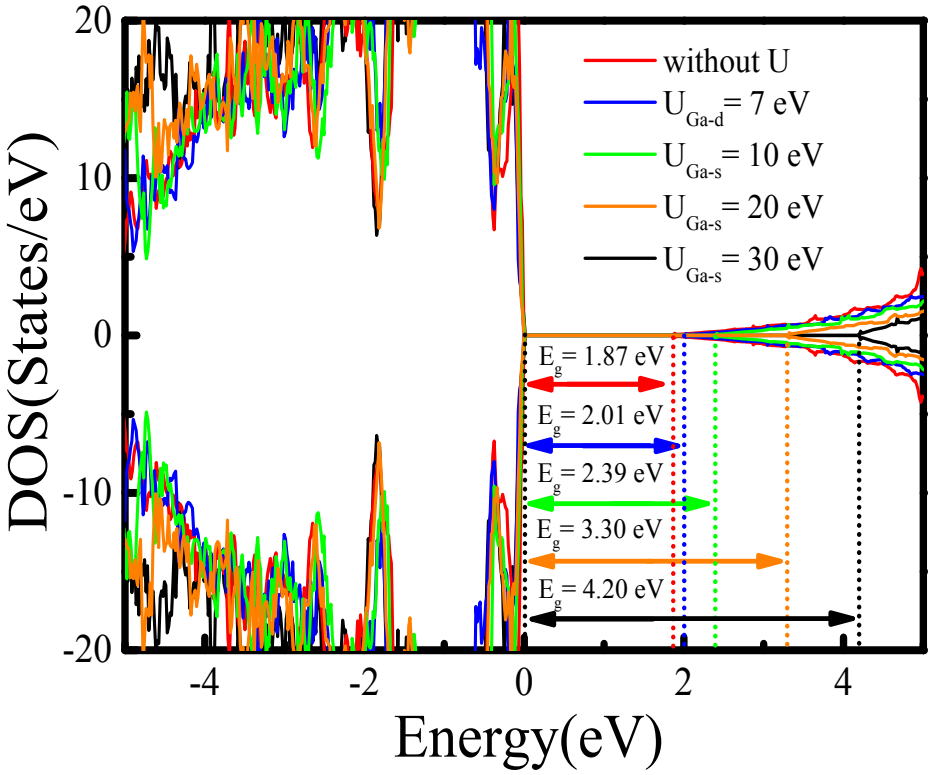

Figure-S1: Total DOS of pure β-Ga_2O_3 with $U_{Ga\text{-}d}$ = 7.0 eV, $U_{Ga\text{-}s}$ = 10.0 eV, $U_{Ga\text{-}s}$ = 20.0 eV, $U_{Ga\text{-}s}$ = 30.0 eV and without U. In the case of using GGA+U method, the $U_{O\text{-}p}$ = 8.5 eV. It is noteworthy that once the $U_{Ga\text{-}s}$ is larger than 30.0 eV, the calculation is very hard to be converged.

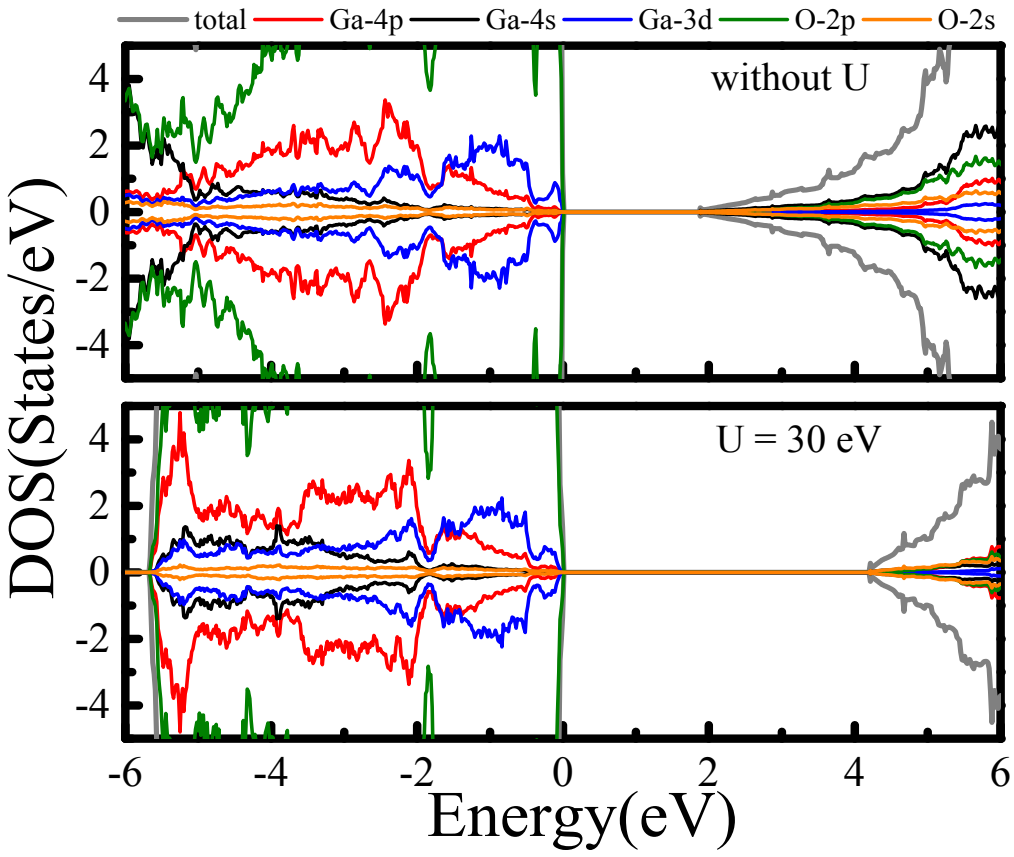

Figure-S2: Projected DOS of pure β-Ga_2O_3 with $U_{Ga\text{-}s}$ = 30.0 eV ($U_{O\text{-}p}$ = 8.5 eV) and without U. In the case without U, it can be seen that the Ga-4s (black line) and the O-2p (green line) are dominating in the bottom of conduction band. In the case of $U_{Ga\text{-}s}$ = 30.0 eV and $U_{O\text{-}p}$ = 8.5 eV, the corresponding states are suppressed to widen the band gap.

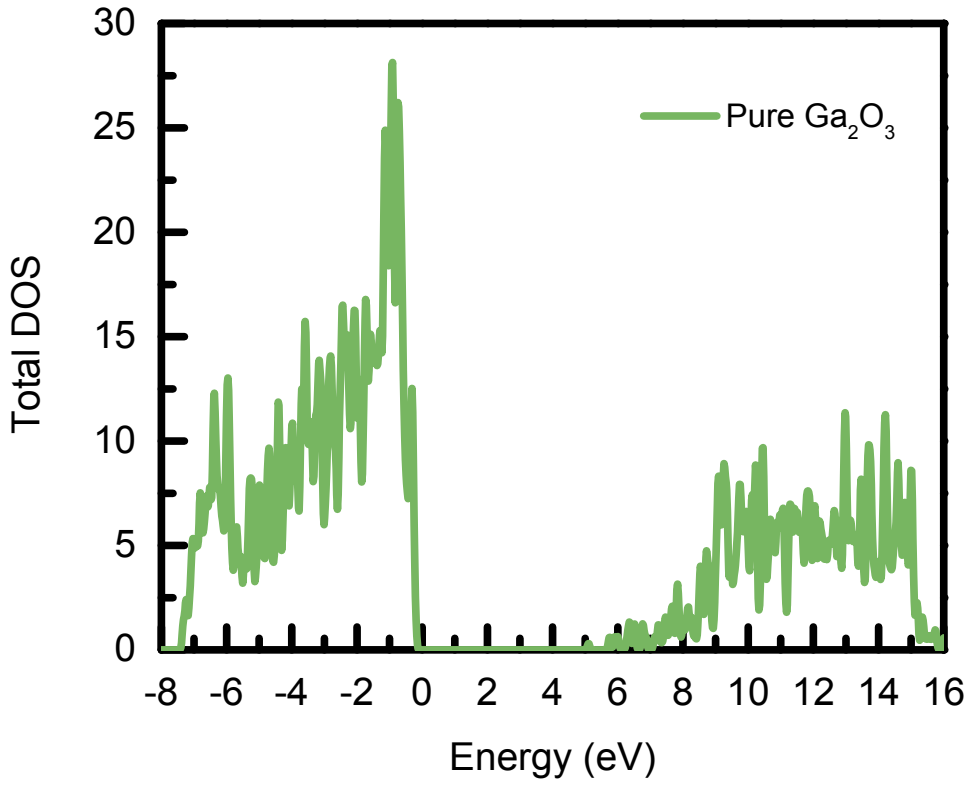

Figure-S3 Calculated TDOS of pure β-Ga_2O_3 using HSE06 functional with a screening parameter $\omega = 0.2 Å^{-1}$ and a big mixing parameter α ($\alpha = 0.45$) for the short-range Hartree-Fock exchange instead of the commonly used value of 0.25 for better fitting the experimental band gaps.

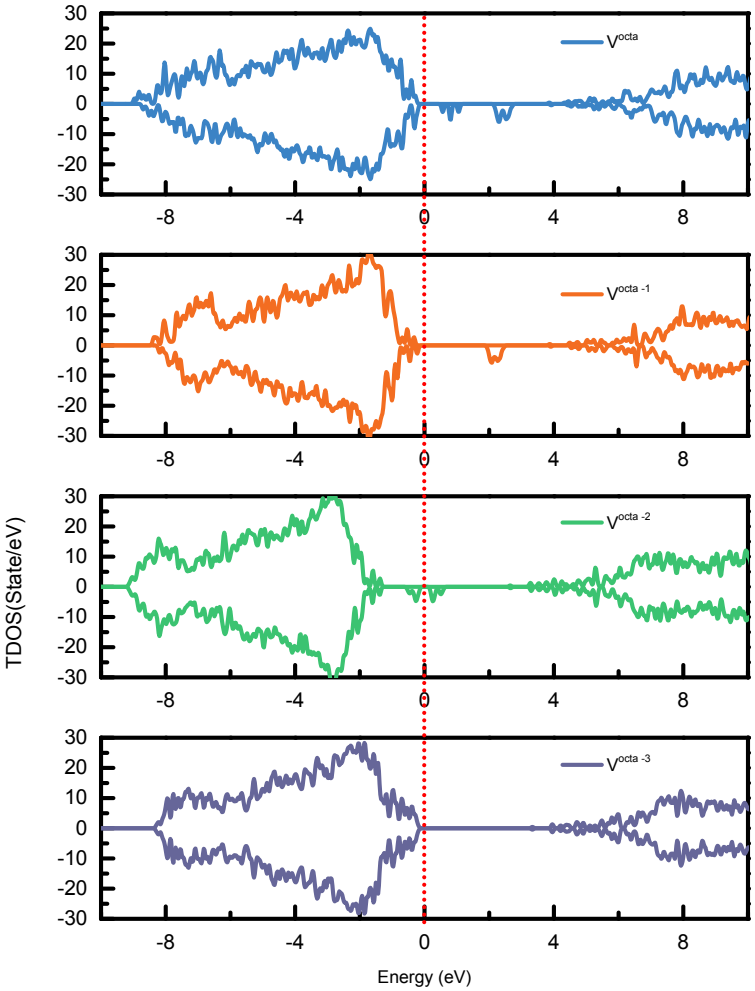

Figure-S4 Calculated TDOS of V^{octa} Ga vacancy in various charge states using HSE06 functional with a screening parameter $\omega = 0.2 Å^{-1}$ and a big mixing parameter α ($\alpha = 0.45$). The local moments induced by the V^{octa} defects in 0, -1, -2, and -3 charge states are 2.457, 1.619, 0.862, and 0 μ_B, respectively.

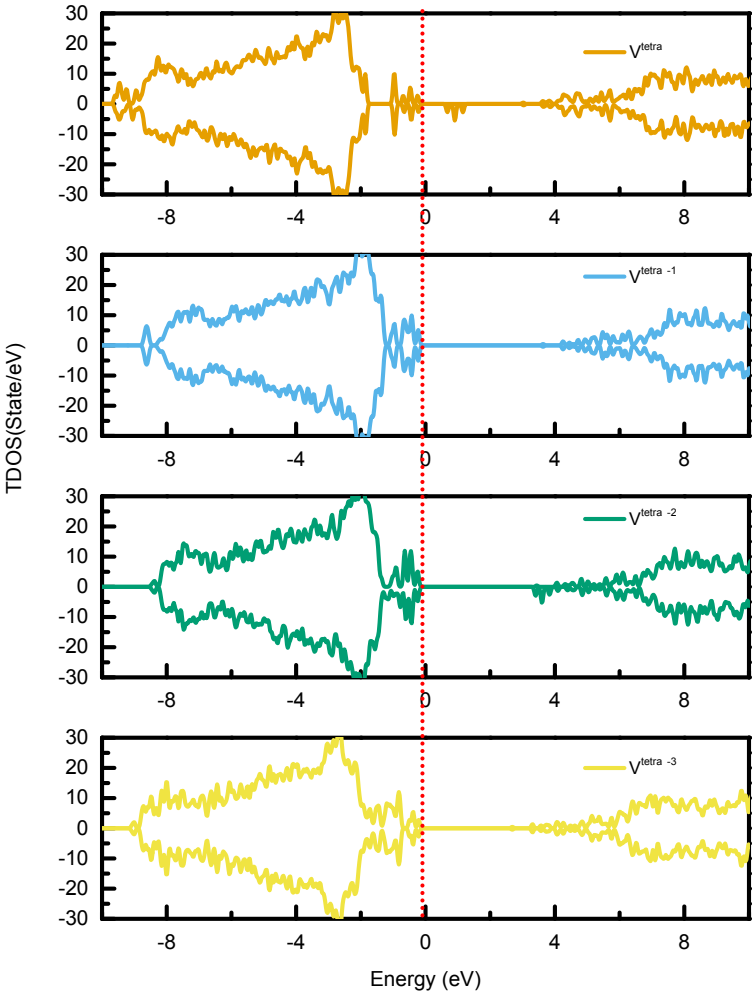

Figure-S5 Calculated TDOS of V^{tetra} Ga vacancy in various charge states using HSE06 functional with a screening parameter $\omega = 0.2 Å^{-1}$ and a big mixing parameter α (α = 0.45). The local moments induced by the V^{octa} defects in 0, -1, -2, and -3 charge states are 0.815, 0, 0.859, and 0 μ_B, respectively.

Table-S2. The magnetic moments of V^{octa} and V^{tetra} with different U.

V^{octa}	Magnetic moments (μ_B)				
	without U	$U_{Ga\text{-}d}$ = 7.0 eV	$U_{Ga\text{-}s}$ = 10.0 eV	$U_{Ga\text{-}s}$ = 20.0 eV	$U_{Ga\text{-}s}$ = 30.0 eV
neutral	2.018	2.014	2.011	2.021	2.034
-1	1.337	1.335	1.335	1.342	1.351
-2	0.680	0.680	0.679	0.683	0.687
-3	0	0	0	0	0

V^{tetra}	Magnetic moments (μ_B)				
	without U	$U_{Ga\text{-}d}$ = 7.0 eV	$U_{Ga\text{-}s}$ = 10.0 eV	$U_{Ga\text{-}s}$ = 20.0 eV	$U_{Ga\text{-}s}$ = 30.0 eV
neutral	0.585	0.679	0.679	0.681	0.685
-1	0	0	0	0	0
-2	0.525	0.625	0.618	0.636	0.690
-3	0	0	0	0	0