

## Supplementary: First principles investigation of electron mobility enhancement of $\beta$ -Ga<sub>2</sub>O<sub>3</sub> doped with Indium

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Table S1 the detailed TDOS of Ga<sub>2</sub>O<sub>3</sub> and In-Ga<sub>2</sub>O<sub>3</sub> near the CBM

Ga <sub>2</sub> O <sub>3</sub>		In-Ga <sub>2</sub> O <sub>3</sub>	
Energy(eV)	TDOS(1/eV)	Energy(eV)	TDOS(1/eV)
1.7874	0	1.7479	0
1.8564	0	1.8169	0
1.9254	0	1.8849	0
1.9954	0.00000096	1.9539	0.0005415
2.0644	0.01676	2.0219	0.009534
2.1334	0.06654	2.0909	0.02959
2.2034	0.1449	2.1589	0.06071
2.2724	0.1986	2.2279	0.1029
2.3424	0.2232	2.2959	0.1561
2.4114	0.2561	2.3649	0.2226
2.4804	0.2997	2.4329	0.3246
2.5504	0.3488	2.5019	0.4201
2.6194	0.4043	2.5709	0.4963
2.6894	0.494	2.6389	0.549

2.7584	0.5401	2.7079	0.5776
2.8274	0.5584	2.7759	0.586
2.8974	0.568	2.8449	0.5851

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The matrix of elastic constants  $C_{ij}$  (GPa) of pure  $\text{Ga}_2\text{O}_3$  (in GPa)

[288.4, 140.2, 171.7, 0, 0, -20.6]

[140.2, 412.6, 123.4, 0, 0, 7.6]

[171.7, 123.4, 401.7, 0, 0, 6.5]

[0, 0, 0, 108.5, 20.4, 0]

[0, 0, 0, 20.4, 82.4, 0]

[-20.6, 7.6, 6.5, 0, 0, 83.2]

The matrix of elastic constants  $C_{ij}$  (GPa) of In- $\text{Ga}_2\text{O}_3$  (in GPa)

[281.8, 130.1, 164.2, 0, 0, -20.2]

[139.1, 403.9, 122.3, 0, 0, 4.7]

[164.2, 122.3, 385.2, 0, 0, 1.7]

[0, 0, 0, 103.1, 18.0, 0]

[0, 0, 0, 18.0, 81.0, 0]

[-20.2, 4.7, 1.7, 0, 0, 75.4]

The matrix of elastic constants  $C_{ij}$  (GPa) of Al- $\text{Ga}_2\text{O}_3$  (in GPa)

[295.8, 143.2, 170.1, 0, 0, -20.3]

[143.2, 419.0, 123.0, 0, 0, 8.1]

[170.1, 123.0, 406.5, 0, 0, 7.3]

[0, 0, 0, 110.7, 19.8, 0]

[0, 0, 0, 19.8, 83.6, 0]

[-20.3, 8.1, 7.3, 0, 0, 84.9]

The matrix of deformation potential of  $\text{Ga}_2\text{O}_3$  (in eV)

[[3.15 0.19 0.12]  
 [0.19 2.16 0.01]  
 [0.12 0.01 3.27]]

The matrix of deformation potential of In-Ga<sub>2</sub>O<sub>3</sub> (in eV)

[[2.88 0.20 0.12]  
 [0.20 2.17 0.02]  
 [0.12 0.02 2.93]]

The matrix of deformation potential of Al-Ga<sub>2</sub>O<sub>3</sub> (in eV)

[[3.29 0.21 0.17]  
 [0.21 2.36 0.00]  
 [0.17 0.00 3.30]]

Table S2. Calculated Frohlich Parameter ( $\alpha$ ) and Schultz Polaron Radius ( $r_f$ ) for Electrons in Ga<sub>2</sub>O<sub>3</sub>, Al-Ga<sub>2</sub>O<sub>3</sub>, In-Ga<sub>2</sub>O<sub>3</sub> at T=300K

	$\alpha$			$r_f$ (Å)		
	Ga <sub>2</sub> O	Al-	In-	Ga <sub>2</sub> O	Al-	In-
	<sub>3</sub>	Ga <sub>2</sub> O <sub>3</sub>	Ga <sub>2</sub> O <sub>3</sub>	<sub>3</sub>	Ga <sub>2</sub> O <sub>3</sub>	Ga <sub>2</sub> O <sub>3</sub>
average	1.16	1.25	1.17	145.8	138.1	142.3
x	1.12	1.23	1.14	148.9	139.0	144.2
y	1.07	1.15	1.05	154.0	144.0	149.7
z	1.25	1.32	1.26	141.1	133.9	136.8