

## Electronic Supplementary Material

### Indium Doping-Assisted Monolayer Ga<sub>2</sub>O<sub>3</sub> Exfoliation for Performance-Enhanced

#### MOSFETs

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**Table S1**  $\Delta E$  (eV/nm<sup>2</sup>) of ML Ga<sub>2</sub>O<sub>3</sub> with different In doping concentrations and atomic configurations, and is defined as the relative energy difference between the In-doped ML Ga<sub>2</sub>O<sub>3</sub> and the pristine ML Ga<sub>2</sub>O<sub>3</sub>. The corresponding structure is presented in Fig. S2.

	$\Delta E$ (eV/nm <sup>2</sup> )
ML GaInO <sub>3</sub> BA'	16.58
ML GaInO <sub>3</sub> AB	17.19
ML GaInO <sub>3</sub> AA'	10.29
ML Ga <sub>1.5</sub> In <sub>0.5</sub> O <sub>3</sub> AB	8.95
ML Ga <sub>1.5</sub> In <sub>0.5</sub> O <sub>3</sub> A	6.52
ML Ga <sub>1.5</sub> In <sub>0.5</sub> O <sub>3</sub> AA'	6.19
ML 13% In-Ga <sub>2</sub> O <sub>3</sub>	3.17
ML 6% In-Ga <sub>2</sub> O <sub>3</sub>	1.65
ML 3% In-Ga <sub>2</sub> O <sub>3</sub>	0.69

**Table S2** Phonon mode-resolved electron mobility of ML Ga<sub>2</sub>O<sub>3</sub>, Ga<sub>1.5</sub>In<sub>0.5</sub>O<sub>3</sub> and GaInO<sub>3</sub>.

Phonon Mode	ML Ga <sub>2</sub> O <sub>3</sub>		ML Ga <sub>1.5</sub> In <sub>0.5</sub> O <sub>3</sub>		ML GaInO <sub>3</sub>	
	x direction	y direction	x direction	y direction	x direction	y direction
ZA	2.85E+03	4.83E+03	2.21E+01	5.26E+01	1.86E+03	3.16E+03
TA	2.00E+05	1.78E+05	1.33E+04	2.31E+04	1.54E+05	1.54E+05
LA	1.57E+05	2.32E+05	4.10E+03	5.25E+03	1.01E+05	1.61E+05
OP1	2.15E+05	2.51E+05	2.93E+05	1.20E+05	7.81E+04	5.66E+04
OP2	1.26E+09	9.33E+08	2.63E+06	7.62E+06	1.13E+08	8.07E+07
OP3	1.29E+09	1.77E+09	1.93E+04	1.92E+04	8.38E+03	9.03E+03
OP4	1.25E+06	1.01E+06	2.22E+05	4.36E+05	2.97E+04	2.14E+04
OP5	7.93E+05	1.40E+06	2.77E+04	1.88E+04	5.09E+08	4.05E+08
OP6	2.17E+05	1.10E+05	7.08E+05	1.95E+06	1.83E+05	3.10E+05
OP7	1.31E+09	2.50E+08	3.14E+05	1.78E+05	9.38E+06	6.02E+06
OP8	1.49E+05	1.11E+05	2.04E+05	2.12E+05	2.23E+04	2.54E+04
OP9	5.36E+05	3.26E+05	3.98E+04	2.90E+04	5.25E+05	4.20E+05
OP10	3.69E+07	2.65E+07	2.36E+05	3.17E+05	2.38E+04	1.96E+04
OP11	3.52E+09	4.67E+09	2.12E+08	2.39E+08	7.10E+06	8.65E+06
OP12	2.15E+10	3.16E+10	1.94E+07	1.50E+07	1.60E+06	2.10E+07
OP13	5.27E+08	3.90E+08	3.69E+07	3.71E+07	6.42E+05	5.36E+06
OP14	4.47E+06	4.78E+06	5.70E+05	4.75E+05	3.21E+05	3.15E+05
OP15	2.44E+07	1.38E+07	1.59E+06	1.29E+06	4.84E+05	3.46E+05
OP16	2.79E+07	2.38E+07	1.32E+05	1.74E+05	5.42E+05	4.64E+05
OP17	5.06E+05	7.99E+05	5.53E+04	7.27E+04	8.49E+03	1.07E+04
OP18	7.17E+06	5.60E+06	4.16E+04	8.18E+04	2.48E+05	1.89E+05
OP19	4.73E+05	1.25E+06	5.05E+04	1.29E+05	2.98E+04	1.32E+06
OP20	1.03E+07	1.51E+07	1.84E+05	2.25E+05	2.15E+06	3.25E+06

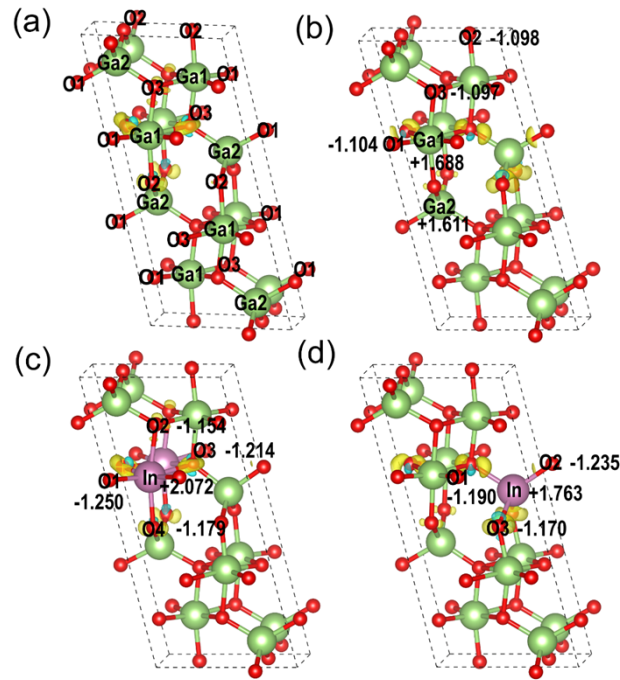
OP21	8.79E+06	1.26E+07	3.85E+06	5.40E+06	3.78E+07	4.56E+07
OP22	2.37E+08	1.50E+08	4.81E+05	6.79E+05	3.41E+06	1.20E+06
OP23	9.69E+06	1.26E+07	2.32E+05	2.49E+05	2.01E+05	2.93E+05
OP24	1.75E+07	3.45E+07	2.48E+05	5.75E+05	6.02E+04	9.49E+04
OP25	6.76E+10	1.23E+11	2.68E+07	3.72E+07	1.10E+07	1.22E+07
OP26	8.42E+07	1.46E+08	4.75E+06	7.17E+06	6.48E+06	8.16E+06
OP27	9.97E+08	1.64E+09	8.93E+06	1.41E+07	1.05E+07	2.27E+07

**Table S3** Phonon mode-resolved hole mobility of ML Ga<sub>2</sub>O<sub>3</sub> and GaInO<sub>3</sub>.

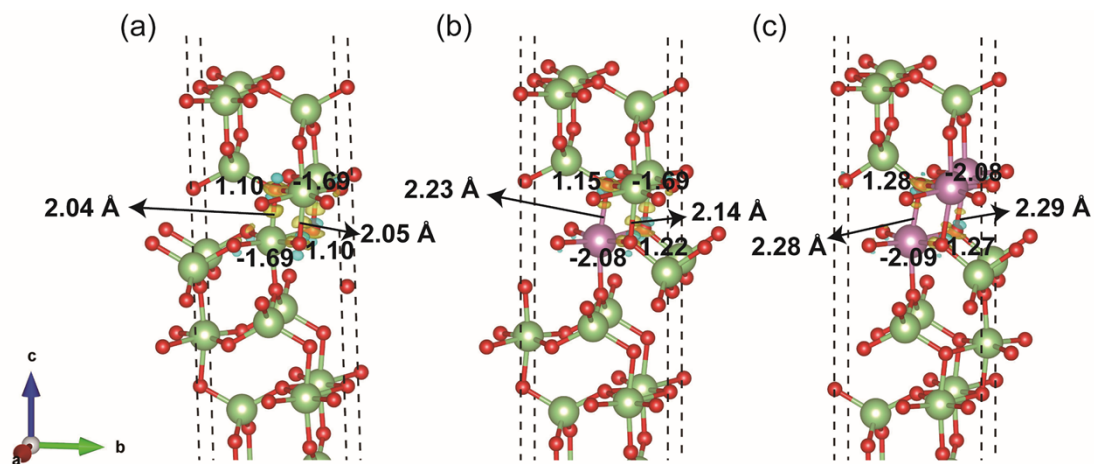
Phonon Mode	ML Ga <sub>2</sub> O <sub>3</sub>		ML GaInO <sub>3</sub>	
	x direction	y direction	x direction	y direction
ZA	8.60E+04	4.83E+03	1.45E+04	1.56E+06
TA	1.25E+05	1.78E+05	4.51E+04	4.29E+06
LA	5.83E+03	2.32E+05	1.91E+03	1.39E+05
OP1	7.71E+03	2.51E+05	6.21E+02	4.91E+04
OP2	8.72E+07	9.33E+08	2.68E+03	1.84E+05
OP3	1.08E+04	1.77E+09	3.75E+02	2.97E+04
OP4	1.46E+04	1.01E+06	5.78E+03	4.89E+05
OP5	1.43E+04	1.40E+06	1.60E+07	1.30E+09
OP6	7.55E+03	1.10E+05	3.69E+03	2.79E+05
OP7	2.08E+06	2.50E+08	5.21E+04	4.38E+06
OP8	1.67E+03	1.11E+05	5.38E+02	4.45E+04
OP9	4.20E+04	8.57E+06	9.69E+04	8.34E+06
OP10	2.39E+06	9.16E+06	2.70E+03	3.01E+05
OP11	5.93E+06	4.40E+05	1.86E+05	1.27E+07
OP12	1.72E+07	6.43E+05	3.67E+04	2.56E+06
OP13	1.28E+07	6.93E+09	1.32E+05	1.15E+07
OP14	1.36E+05	8.07E+05	1.04E+05	7.11E+06
OP15	5.44E+06	1.00E+06	2.81E+04	1.98E+06
OP16	4.06E+05	1.18E+06	7.94E+03	4.33E+05
OP17	2.63E+03	5.91E+05	7.93E+02	4.81E+04
OP18	1.55E+05	1.75E+08	2.44E+05	1.41E+07
OP19	8.61E+03	1.25E+05	5.24E+03	2.61E+05
OP20	1.70E+05	3.42E+06	2.41E+04	1.50E+06
OP21	1.33E+05	2.01E+08	6.03E+06	4.62E+08
OP22	1.87E+07	5.77E+08	1.64E+06	7.77E+07
OP23	2.26E+06	1.31E+09	7.76E+04	4.42E+06
OP24	4.29E+04	1.28E+09	1.54E+04	8.20E+05
OP25	3.02E+09	1.14E+07	6.72E+06	6.81E+08
OP26	7.05E+05	5.62E+08	3.37E+05	7.02E+06
OP27	1.99E+07	3.77E+07	2.30E+07	3.83E+08

**Table S4** Benchmark of the device performances of the n-type sub-5 nm In-doping ML Ga<sub>2</sub>O<sub>3</sub> MOSFETs against the ITRS requirements for the LP application.

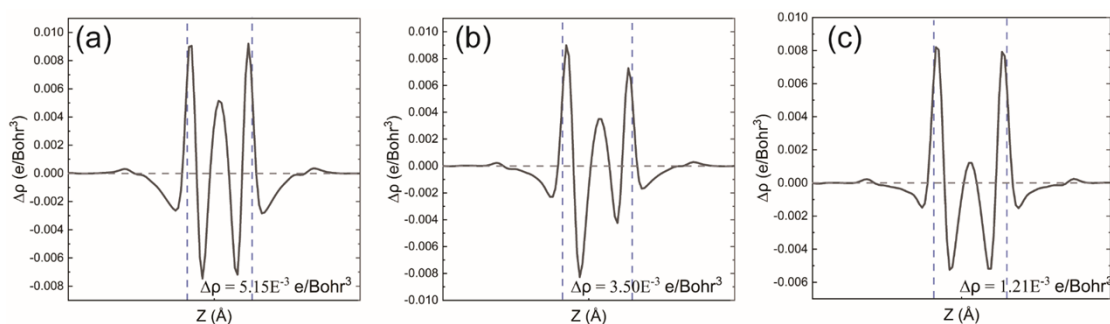
	direction	In-doping concentration	$I_{on}$ ( $\mu\text{A}/\mu\text{m}$ )	SS (mV/dec)	$I_{on}/I_{off}$	$C_g$ (fF/ $\mu\text{m}$ )	$\tau$ (ps)	PDP (fJ/ $\mu\text{m}$ )
LP	x-direction	pristine	390	72	$7.8 \times 10^6$	0.193	0.317	0.034
		3.3 %	475	71	$9.5 \times 10^6$	0.195	0.262	0.035
		6.7 %	575	69	$1.2 \times 10^7$	0.194	0.216	0.035
		10 %	638	69	$1.3 \times 10^6$	0.190	0.191	0.036
		20 %	744	66	$1.5 \times 10^6$	0.188	0.162	0.039
	y-direction	pristine	155	76	$3.1 \times 10^6$	0.202	0.836	0.029
		5 %	350	70	$7.0 \times 10^6$	0.203	0.371	0.032
		10 %	375	70	$7.5 \times 10^6$	0.203	0.347	0.033
		20 %	527	68	$1.1 \times 10^7$	0.207	0.252	0.038
		ITRS <sup>2028</sup>	$L_g = 5.9 \text{ nm}$	295		$5.9 \times 10^6$	0.690	1.493



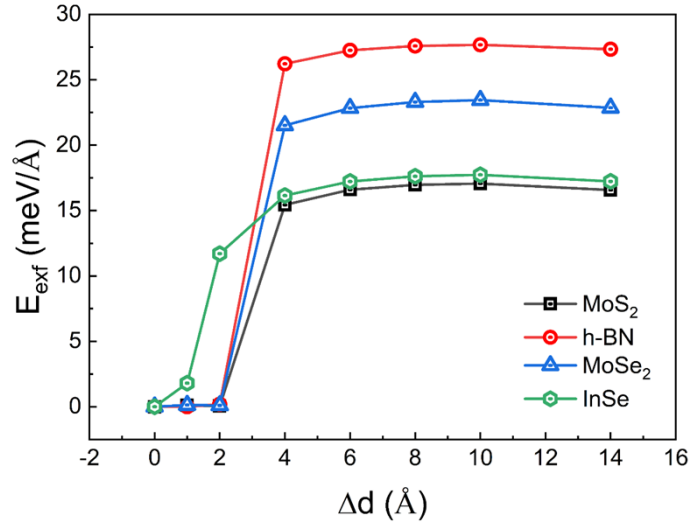
**Figure S1** Charge density difference (equivalence plane is  $0.02 \text{ e}/\text{\AA}^3$ ) and Bader charge analysis for pure and In-doped  $\beta\text{-Ga}_2\text{O}_3$  at the tetrahedral and octahedral Ga atom site.



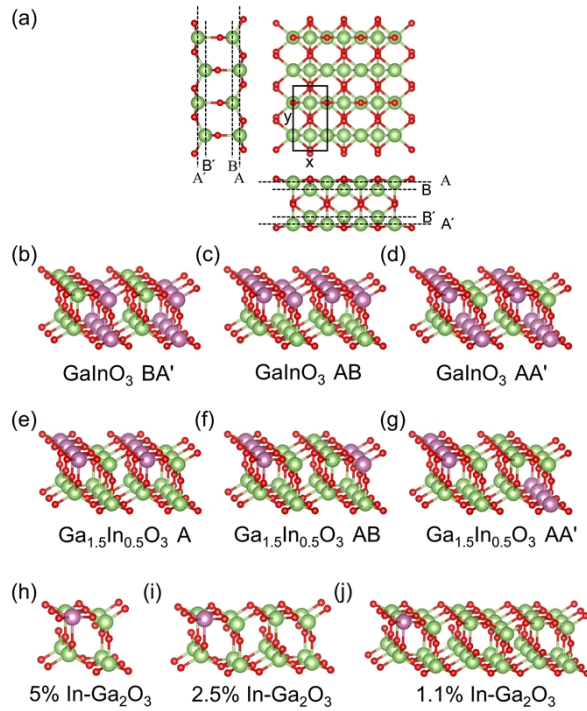
**Figure S2** Charge density difference isosurface distribution of pure (a) and In-doped  $\beta$ - $\text{Ga}_2\text{O}_3$  with different configurations (b), (c), the yellow and cyan regions denote the gain and loss of electrons, respectively, the isosurface value was set to  $0.01e/\text{\AA}^3$ . The In/Ga-O bond length as well as the Bader charge of the interface bonding atoms are labeled for comparison.



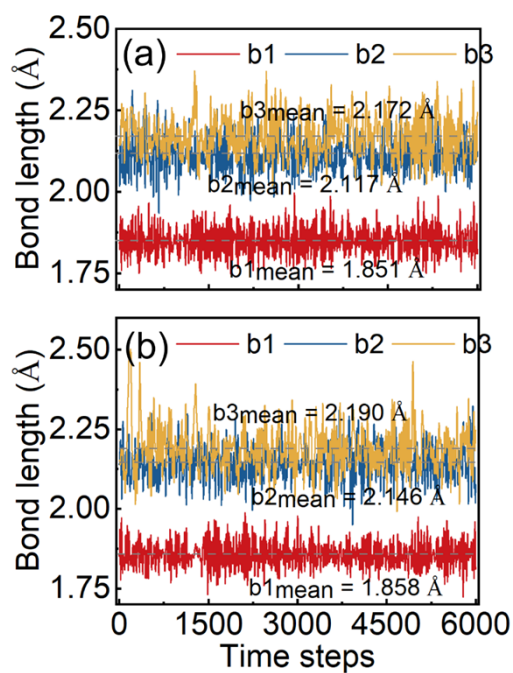
**Figure S3** Charge transfer of pure (a) and In-doped  $\beta$ - $\text{Ga}_2\text{O}_3$  with different configurations (b), (c) along c direction, the blue line represents the plane of outer Ga atom as labeled in Fig. S2.



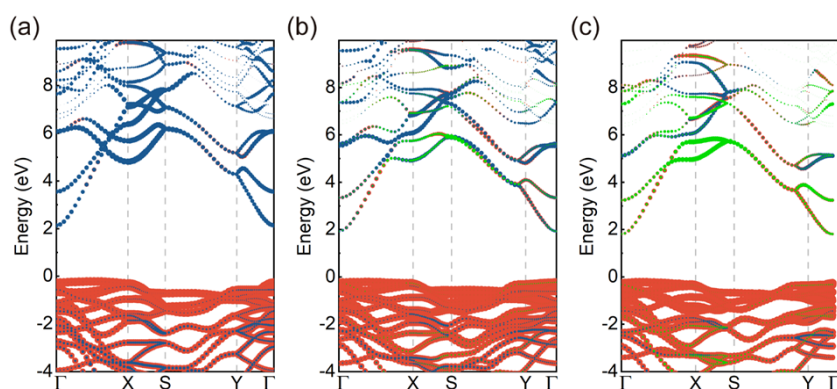
**Figure S4** Single-side exfoliation energy as a function of exfoliation distance of representative van der Waals 2D materials.



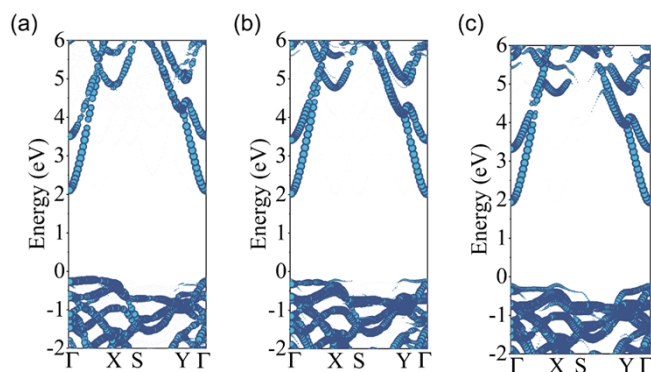
**Figure S5** (a) Top and side views of pristine ML  $\text{Ga}_2\text{O}_3$ , the crystal plane where the Ga atom located is labeled as ABB'A' pattern from top to bottom layers. (b), (c), and (d) are ML  $\text{GaInO}_3$  (20% In concentration) with different configurations, it is noted that (c) possesses a Janus structure. (e), (f), and (g) are ML  $\text{Ga}_{1.5}\text{In}_{0.5}\text{O}_3$  (10% In concentration) with different configurations. Low In concentration-doped ML  $\text{Ga}_2\text{O}_3$  with In concentration of (h) 5 %, (i) 2.5 %, and (j) 1.1 %.



**Figure S6** Bond length as a function of time for ML (a)  $\text{Ga}_{1.5}\text{In}_{0.5}\text{O}_3$  and (b)  $\text{GaInO}_3$  at 300 K in a NVT ensemble with AIMD simulation.

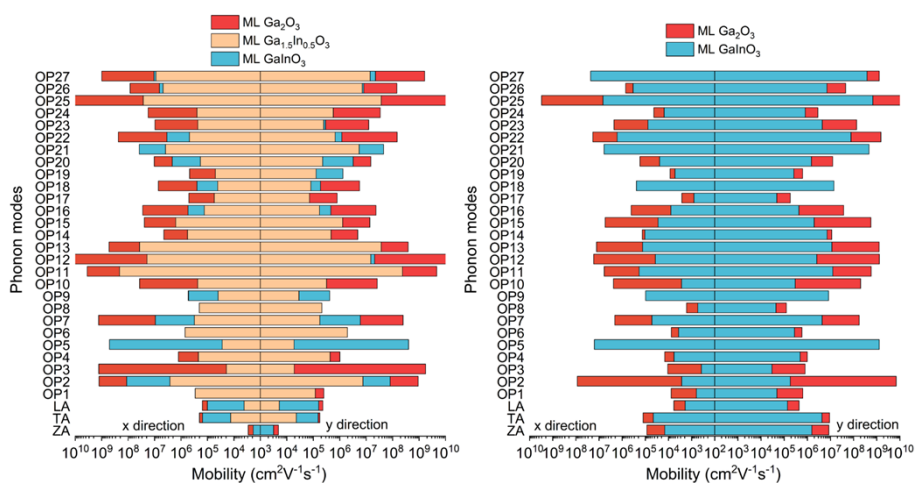


**Figure S7** Element-projected band structure of (a) ML  $\text{Ga}_2\text{O}_3$ , (b) ML  $\text{Ga}_{1.5}\text{In}_{0.5}\text{O}_3$  and (c) ML  $\text{GaInO}_3$ , the contribution from Ga, O, and In are presented by blue, red, and green colors, respectively.

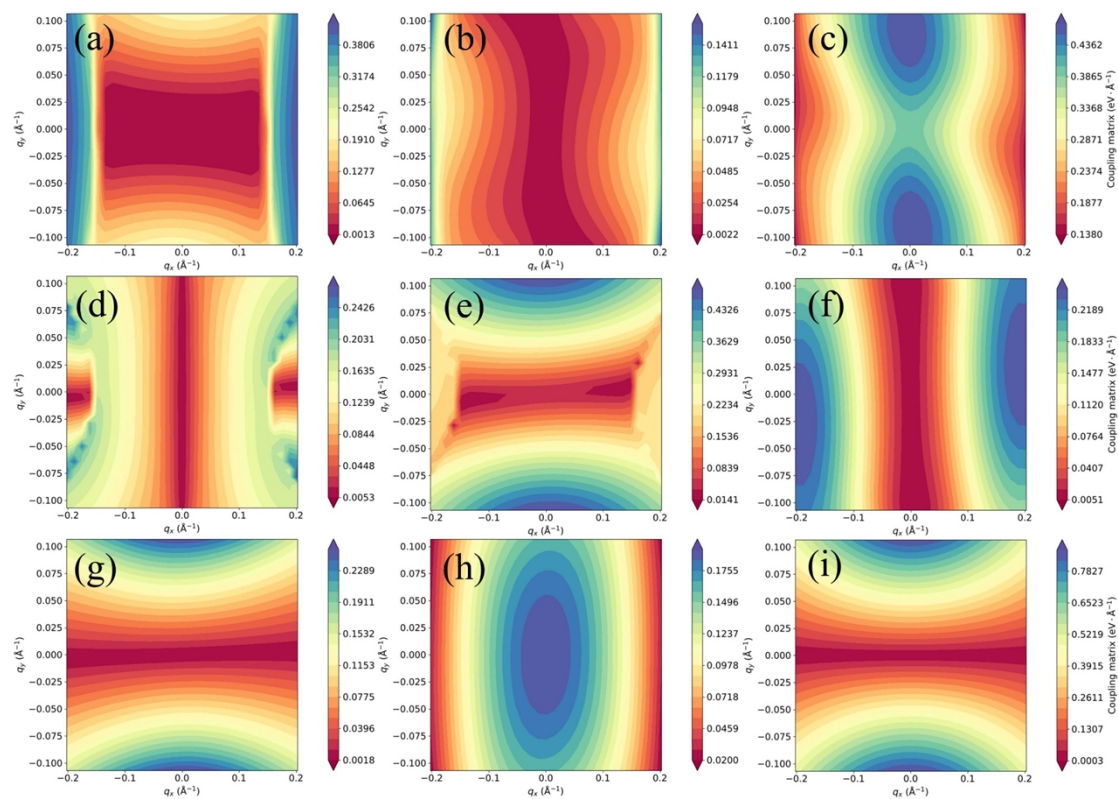


**Figure S8** Unfolded band structures of In-doped ML  $\text{Ga}_2\text{O}_3$  with In concentration of (a) 1.1 %, (b) 2.2 %, and (c) 4.4 %.

2.5 %, and (c) 5 %, respectively.

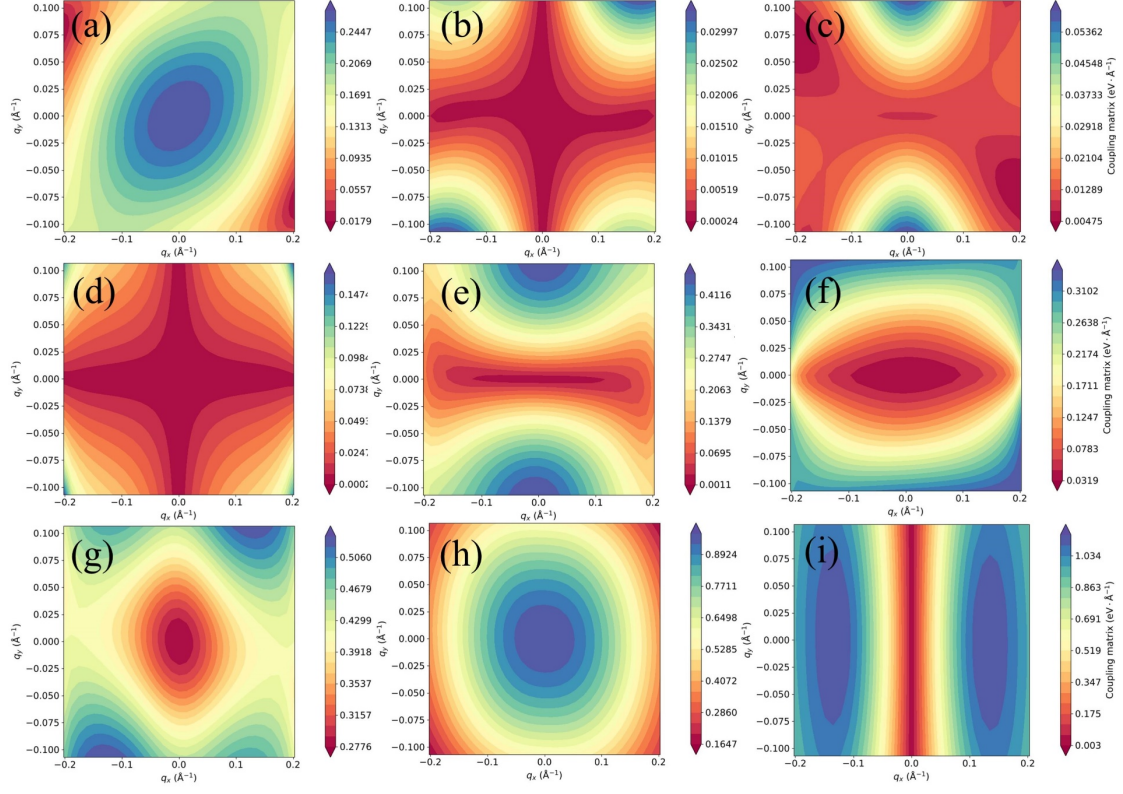


**Figure S9** Phonon mode-resolved electron (a) and hole mobility (b) of pristine and In-doped ML  $\text{Ga}_2\text{O}_3$ .

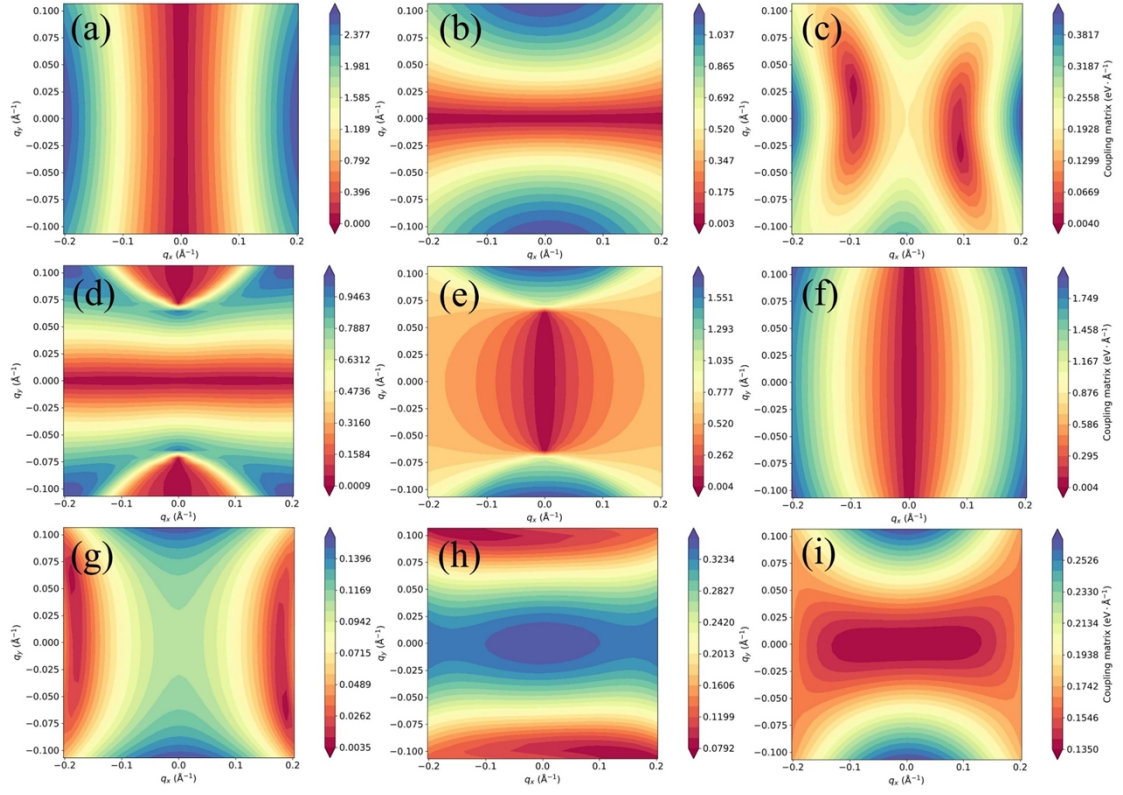


**Figure S10** The EPC matrix elements of the OP1~OP9 for ML  $\text{Ga}_{1.5}\text{In}_{0.5}\text{O}_3$  at the CBM.

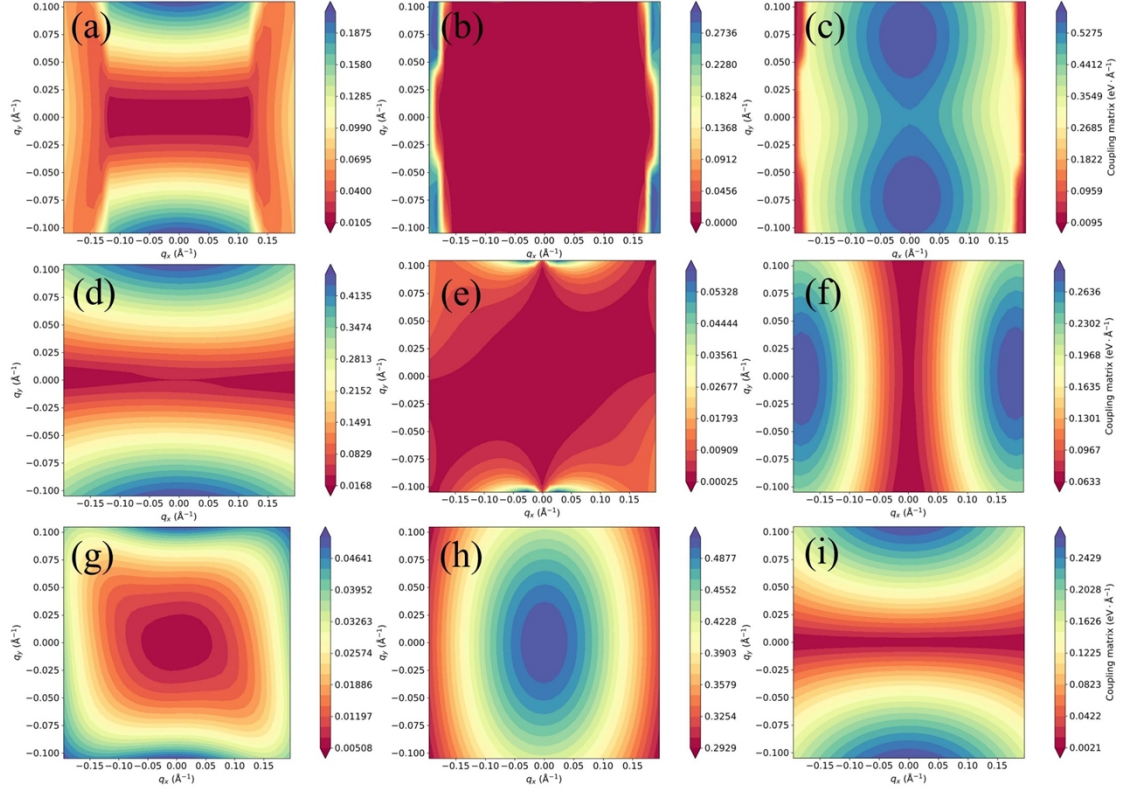




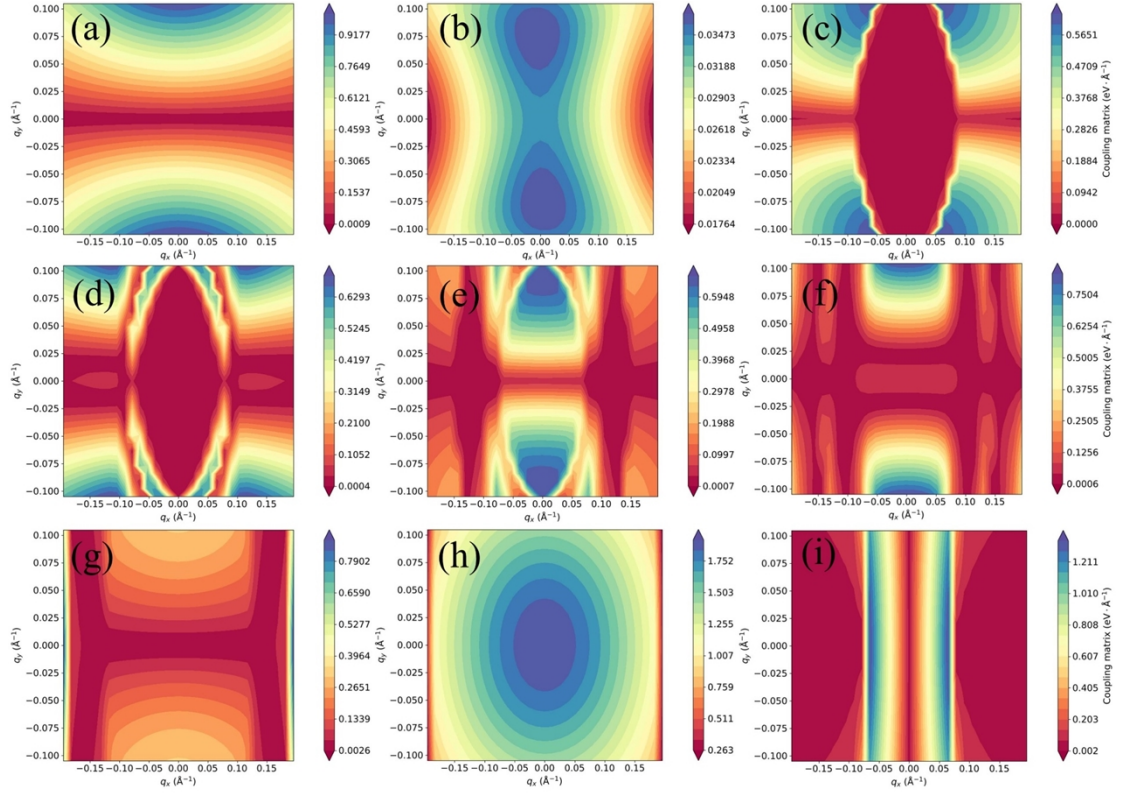
**Figure S11** The EPC matrix elements of the OP10~OP18 for ML  $\text{Ga}_{1.5}\text{In}_{0.5}\text{O}_3$  at the CBM.



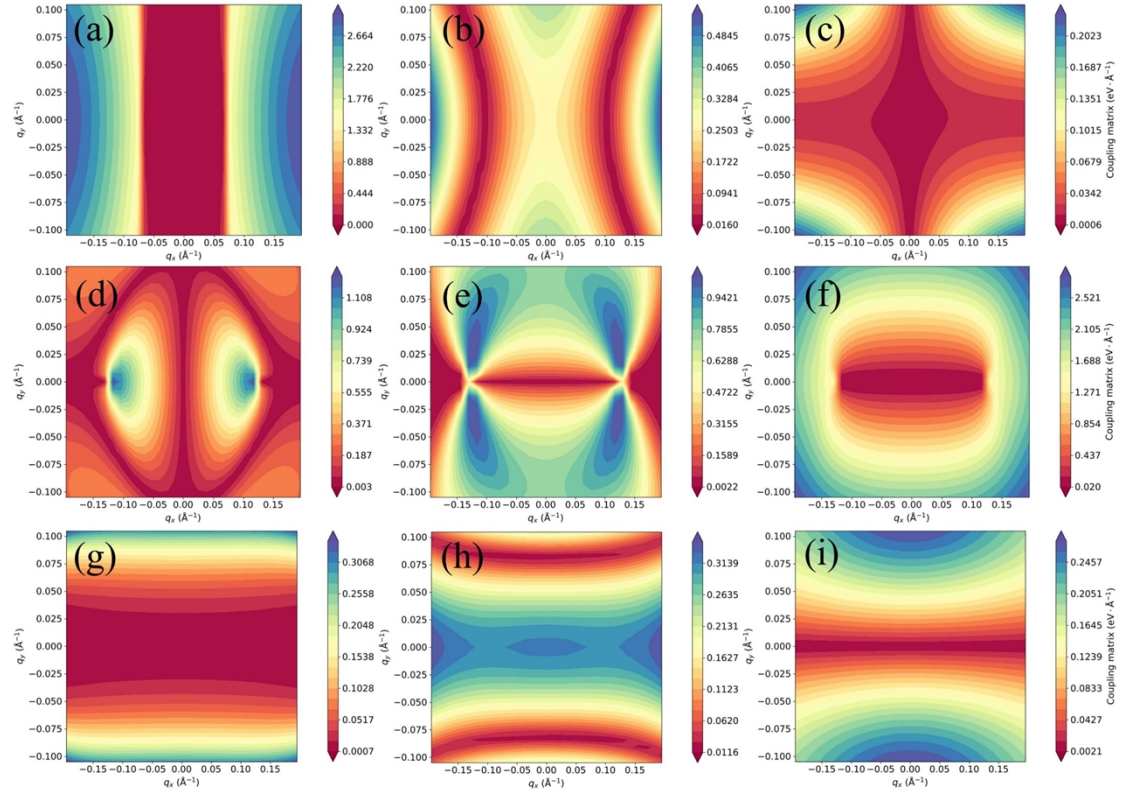
**Figure S12** The EPC matrix elements of the OP19~OP27 for ML  $\text{Ga}_{1.5}\text{In}_{0.5}\text{O}_3$  at the CBM.



**Figure S13** The EPC matrix elements of the OP1~OP9 for ML GaInO<sub>3</sub> at the CBM.



**Figure S14** The EPC matrix elements of the OP10~OP18 for ML GaInO<sub>3</sub> at the CBM.



**Figure S15** The EPC matrix elements of the OP19~OP27 for ML GaInO<sub>3</sub> at the CBM.