

Supplementary Information for

Nontrivial role of polar optical phonons in limiting electron mobility of two-dimensional Ga₂O₃ from first-principles

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S. RESULTS AND DISCUSSIONS

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Table.S1. The matrix of elastic constants for bulk and 2D Ga₂O₃ (in GPa)

		C_{11}	C_{12}	C_{13}	C_{15}	C_{22}	C_{23}	C_{25}	C_{33}	C_{35}	C_{44}	C_{46}	C_{55}	C_{66}
Bulk Ga ₂ O ₃	Cal.	222.9	119.6	139.4	-17.1	338.8	81.4	9.8	326.6	7.3	54.6	19.8	61.4	87.3
	Cal. ¹	220.5	116.4	128.3	-17.3	329.5	79.0	11.4	326.8	7.2	50.0	18.1	66.1	91.5
	Exp. ²	242.8	128.0	160.0	-1.6	343.8	70.9	0.4	347.4	1.0	47.8	5.6	88.6	104.0
ML Ga ₂ O ₃	Cal.	0.24	0.63	6.56	0.15	127.7	0.87	0.61	87.02	2.89	4.61	1.21	0.45	0.44
	Cal. ³	1.57	0.33	9.80	0.42	124.78	0.21	0.21	79.61	0.40	1.72	0.15	0.06	0.34
BL Ga ₂ O ₃	Cal.	19.47	0.64	0.67	0.01	193.39	0.45	0.98	159.18	0.56	24.02	0.34	1.09	1.35
	Cal. ³	17.57	1.05	7.20	1.39	187.38	4.43	1.35	134.77	1.18	24.37	0.67	0.97	2.63

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