

Supporting Information for
Cutting Ultrathin Gallium Oxide Nanoribbons
into Nanoplates having Single Unit-Cell Thickness

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Experimental

TEM, HRTEM images and EDS spectrum were recorded with a JEOL 2100F unit operated at 200 kV. The samples for TEM study were prepared by drop casting nanomaterials dispersed in methylene chloride on carbon-coated copper grids. The TEM studies were performed on as-prepared samples without employing size-selection process. Powder XRD patterns were obtained on a Rigaku Max-2200 with filtered $\text{Cu}_{\text{K}\alpha}$ radiation. X-ray photoelectron spectroscopy (XPS) was obtained using a Thermo VG and Monochromatic $\text{Al-K}\alpha$ radiation. PL studies were performed using Jasco-FP6200.

Figure S1. TEM image (a) of the assembled nanoplates and their HR-TEM image (b).

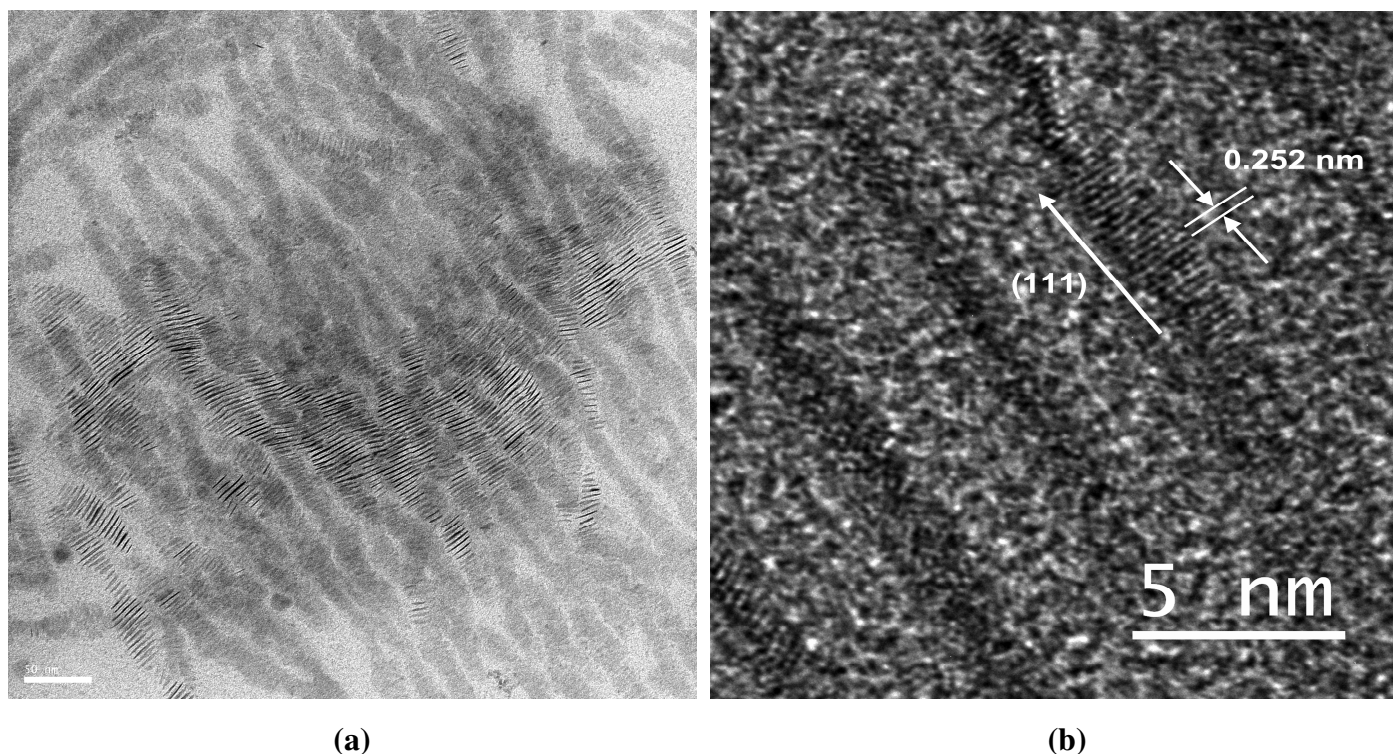


Figure S2. The analysis of the low angle –XRPD pattern (in Figure 3C of text) of nanoplates

2 theta (°)	observed distance(Å)	theoretical distance(Å)
7.2	12.3	12.3 (d/3)
9.6	9.2	9.2 (d/4)
12.0	7.4	7.4 (d/5)
14.4	6.2	6.1 (d/6)

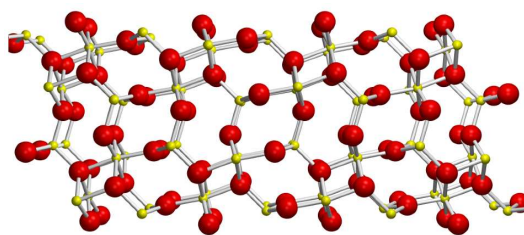
$$\mathbf{d = 36.8 \text{ \AA}}$$

Simulation Method

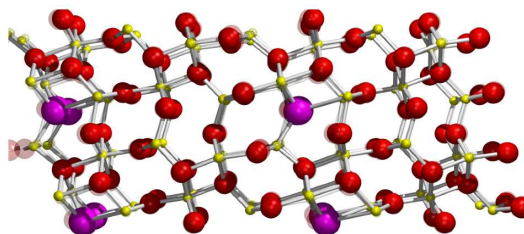
The VASP code¹ was used for planewave pseudopotential calculations based on density functional theory. The exchange-correlation part of electron-electron interaction was described by local density approximation² and electron-ion interaction was described by projected augmented method.³ Electron wavefunctions were expanded by planewaves up to kinetic energy cutoff of 250 eV. The simulated unit cell⁴ has monoclinic structure with lattice parameters of $a = 12.23 \text{ \AA}$, $b = 3.04 \text{ \AA}$, $c = 5.80 \text{ \AA}$ and $\beta = 103.7^\circ$, which contains 4 Ga atoms and 12 O atoms. We used $1 * 4 * 2$ Monkhorst-Pack mesh⁵ for the k-point sampling. For the structure relaxation, we used conjugate-gradient algorithm, where stopping criteria was maximal force on atoms of $2 * 10^{-2} \text{ eV/\AA}$.

References

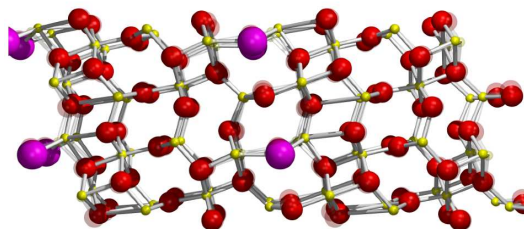
1. Kresse, G.; J. Furthmüller, J. *Comput. Mat. Sci.* **1996**, 6, 15.
2. Perdew, J. P.; Zunger, A. *Phys. Rev. B* **1981**, 23, 5048.
3. (a) Blöchl, P. E. *Phys. Rev. B* **1994**, 50, 17953. (b) Joubert, D.; Kresse, G. *Phys. Rev. B* **1999**, 59, 1758.
4. Geller, S. *J. Chem. Phys.* **1960**, 33, 676.
5. Monkhorst, H. J.; Pack, J. D. *Phys. Rev. B* **1976**, 13, 5188.



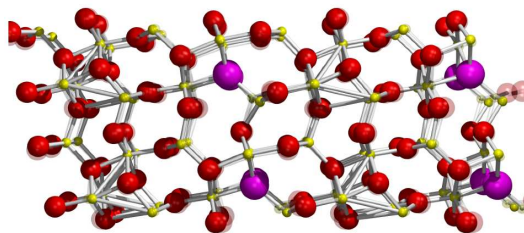
Ga-O1: 1.84, 1.95 Å
Ga-O2: 1.85, 1.93 Å
Ga-O3: 1.88, 2.01 Å



Ga-S1: 2.14, 2.26 Å



Ga-S2: 2.16, 2.22 Å



Ga-S3: 2.14, 2.26 Å