Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary information

Synthesis, oxide formation and dielectric properties of amorphous aluminium oxide using a chimie douce solution precursor route

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Crystal data and structure refinement

Empirical formula	C21 H30 Al N3 O18	
Formula weight	639.46	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 12.159(1) Å	a= 90°.
	b = 17.395(2) Å	b= 106.62(1)°.
	c = 15.406(2) Å	g = 90°.
Volume	3122.3(6) $Å^3$	
Z	4	
Density (calculated)	1.360 Mg/m^3	
Absorption coefficient	0.145 mm^{-1}	
F(000)	1336	
Crystal size	0.400 x 0.180 x 0.040 mm^3	
Theta range for data collection	2.777 to 25.350°.	
Index ranges	-14<=h<=14, -20<=k<=20, -11<=l<=18	
Reflections collected	5911	
Independent reflections	2858 [R(int) = 0.0495]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.994 and 0.944	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	2858 / 4 / 215
Goodness-of-fit on F^2	0.841
Final R indices [I>2sigma(I)]	R1 = 0.0582, wR2 = 0.1270
R indices (all data)	R1 = 0.1716, wR2 = 0.1584
Extinction coefficient	n/a
Largest diff. peak and hole	0.496 and -0.230 e.Å^{-3}

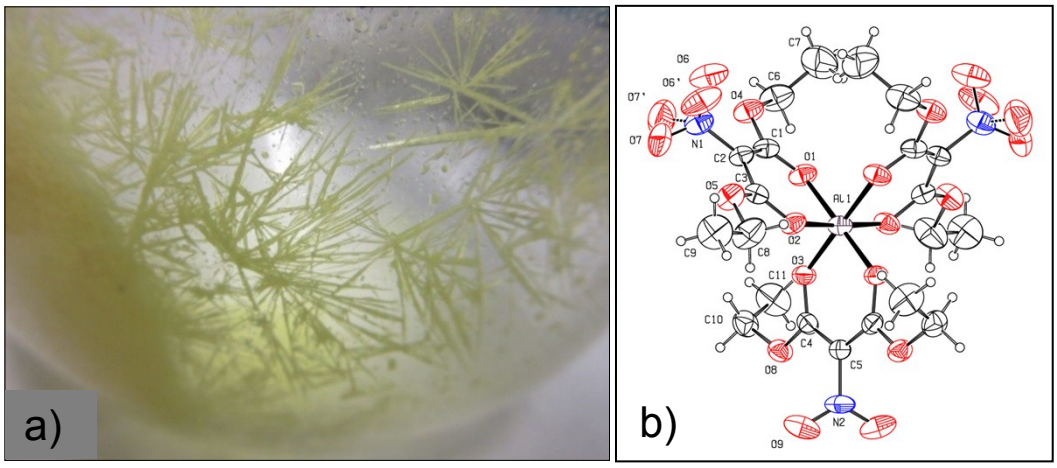

Fig. S1: a) Photography of tris[(diethyl-2-nitromalonato)]aluminum(III)-crystals. b) Single crystal structure of tris(diethyl-2-nitromalonato)aluminum. ORTEP-illustration. Vibrational ellipsoids are given with 30 % probability. O-Al-bond length (185-188 pm); O-Al-O-bond angle (90± 3°).

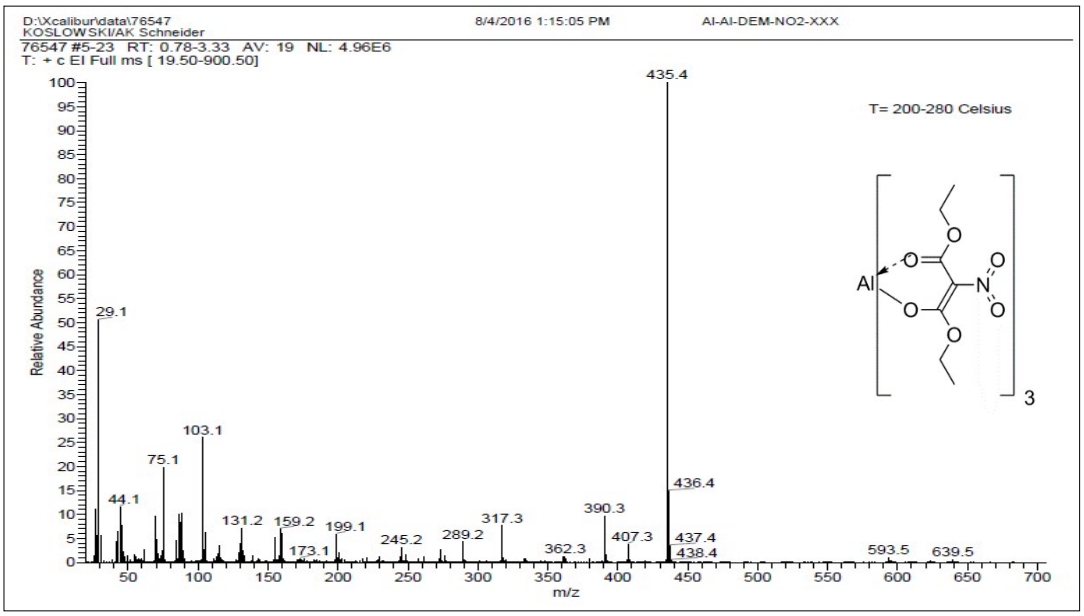

Fig. S2: Mass spectrum (MS-EI) of tris[(diethyl-2-nitromalonato)]aluminum(III) (overview).

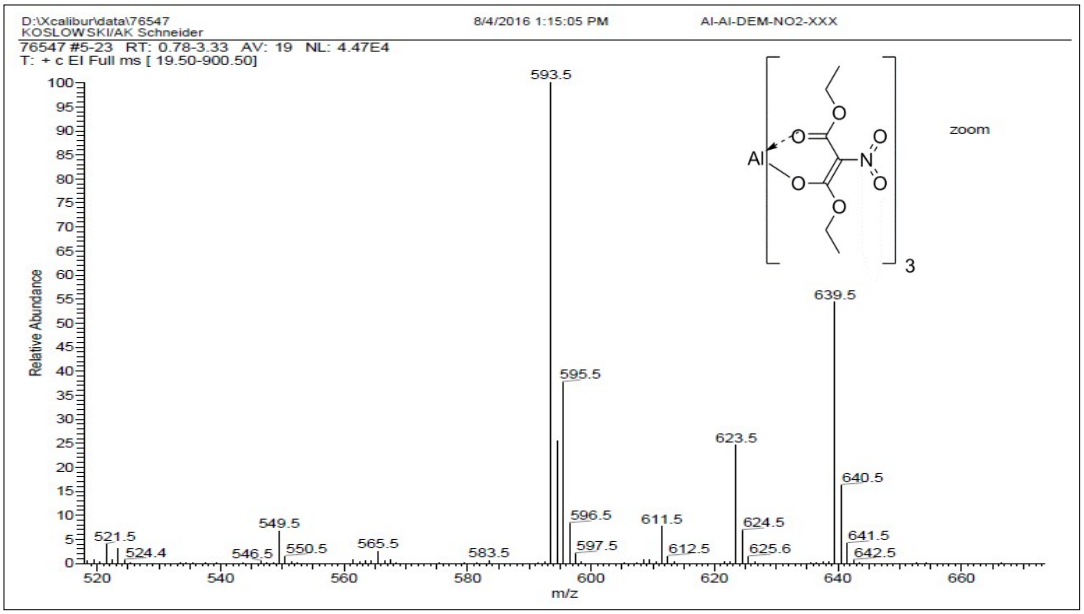

Fig. S3: Mass spectrum (MS-EI) of tris[(diethyl-2-nitromalonato)]aluminum(III) (zoom-in).

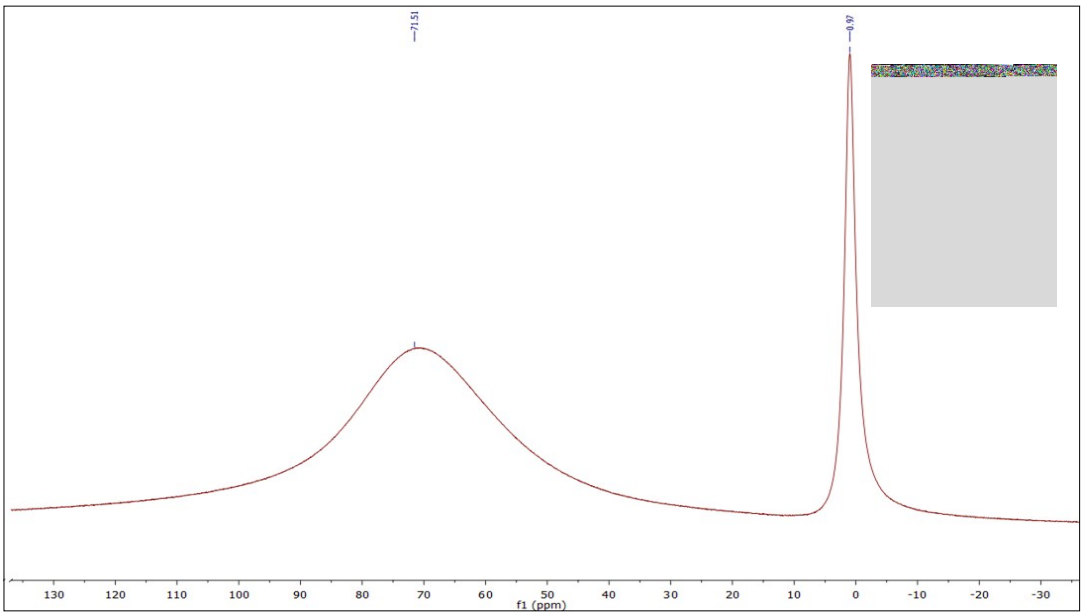

Fig. S4: ^{27}Al-NMR-spectrum ($CDCl_3$) of tris[(diethyl-2-nitromalonato)]aluminum(III).

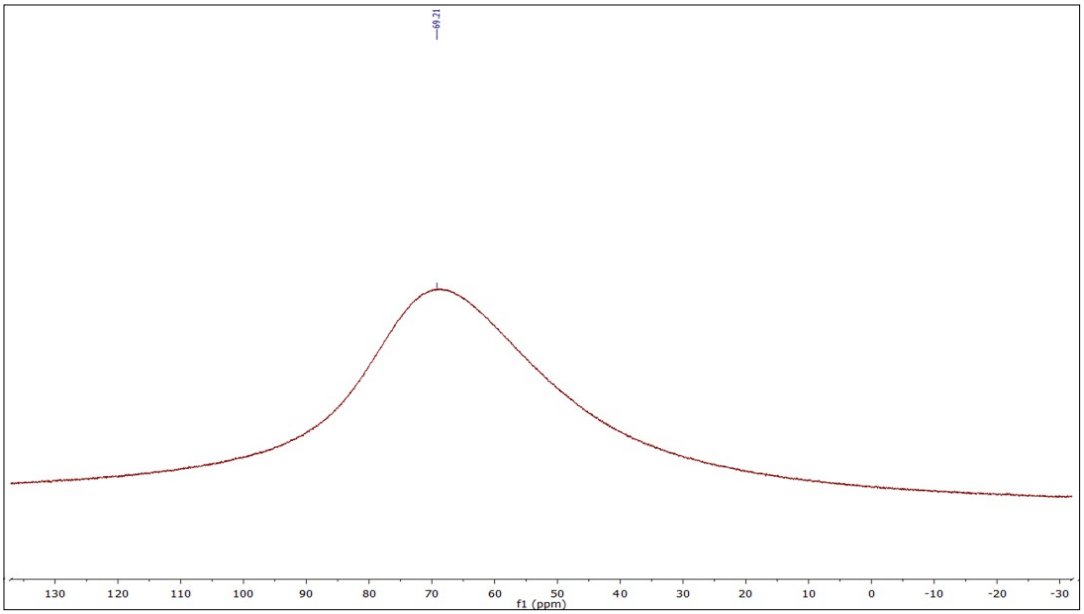

Fig. S5: ^{27}Al-NMR-spectrum of empty crucible.

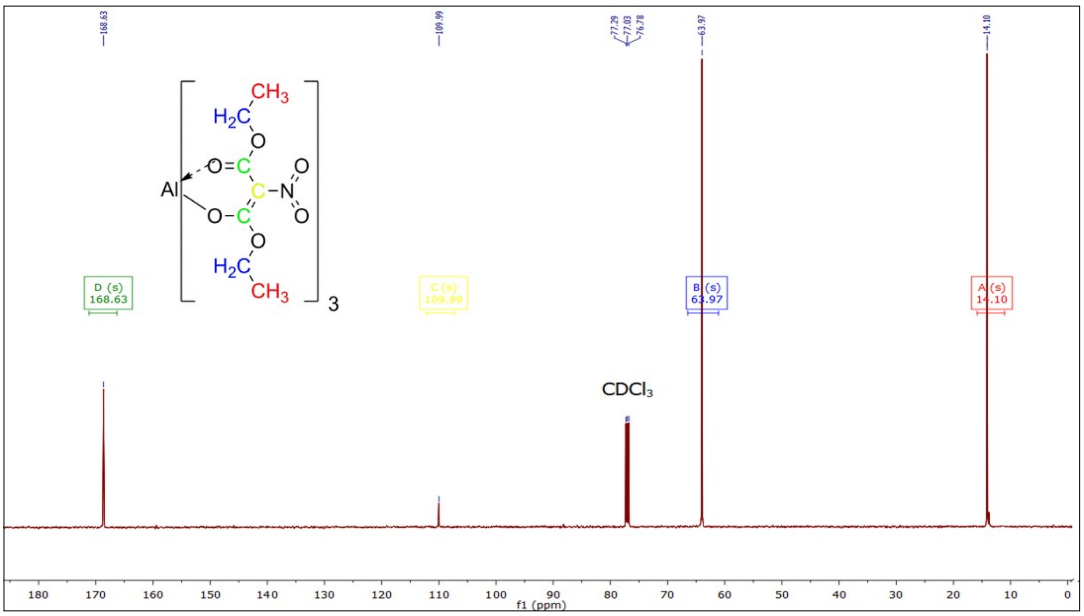

Fig. S6: ^{13}C-NMR-spectrum ($CDCl_3$) of tris[(diethyl-2-nitromalonato)]aluminum(III).

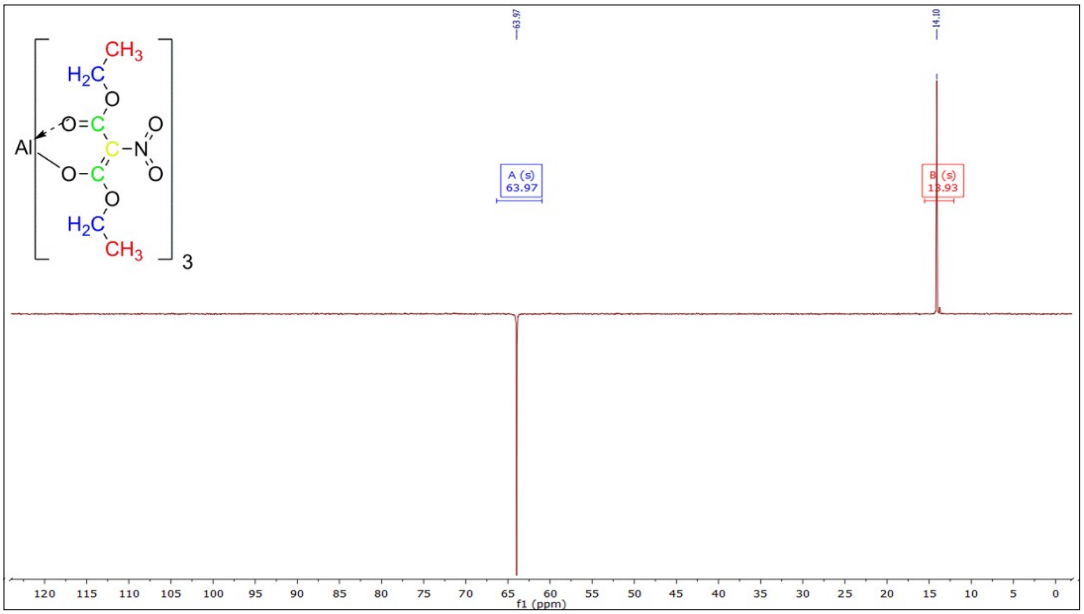

Fig. S7: DEPT-spectrum ($CDCl_3$) of tris[(diethyl-2-nitromalonato)]aluminum(III).

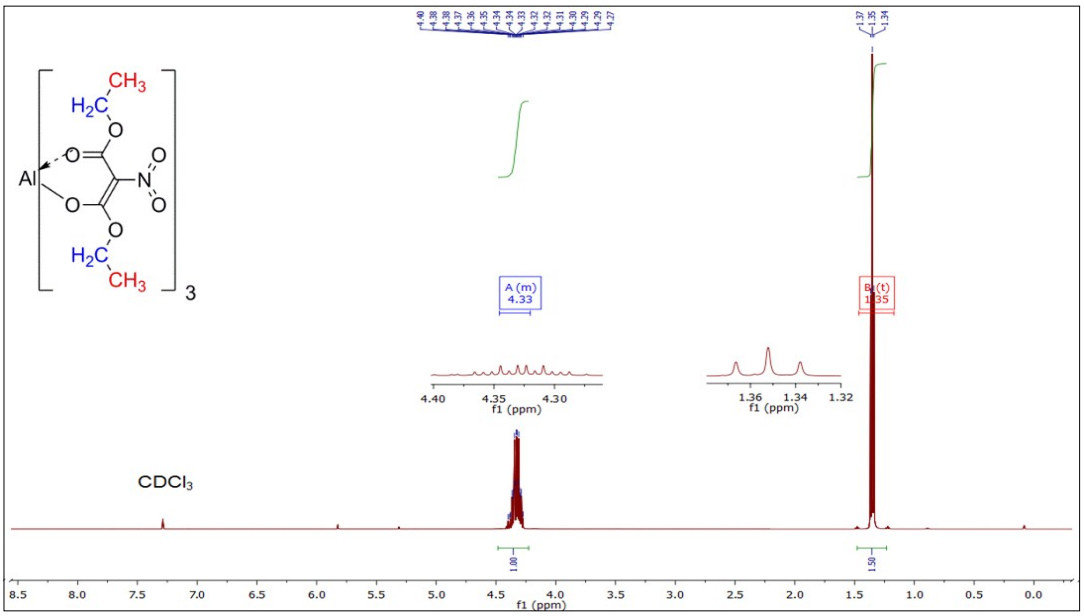

Fig. S8: ^{1}H-NMR-spectrum ($CDCl_3$) of tris[(diethyl-2-nitromalonato)]aluminum(III).

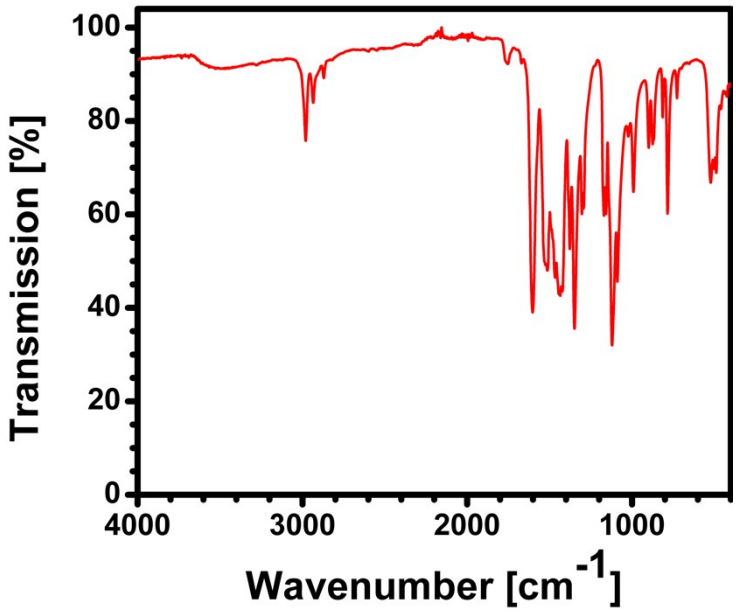

Fig. S9: FTIR-spectrum of tris[(diethyl-2-nitromalonato)]aluminum(III).

Tab S1: Characteristic vibrational bonds of tris[(diethyl-2-nitromalonato)]aluminum(III).

wavenumber / cm^{-1}	vibrational type	chemical compound

2979 /2934 /2870	ν ($-CH_3$) / ν ($-CH_2-$)	saturated carbohydrate
1602 / 1513	ν_{as} ($RCOO^-$)	carbonyl compound
1435	ν_s ($-RCOO^-$)	carbonyl compound
1348	ν ($C-NO_2$)	nitro compound
784	ν (C=C)	alkene
522	ν (Al-O)	metal oxide

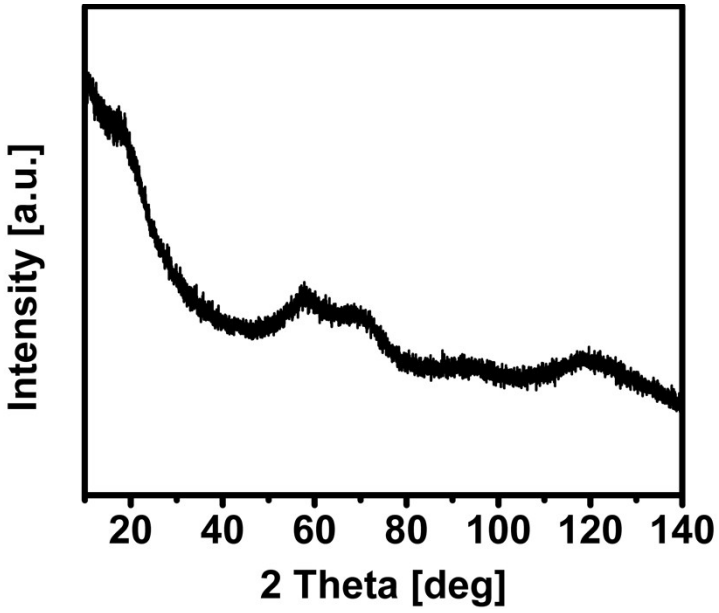

Fig. S10: XRD of empty crucible.

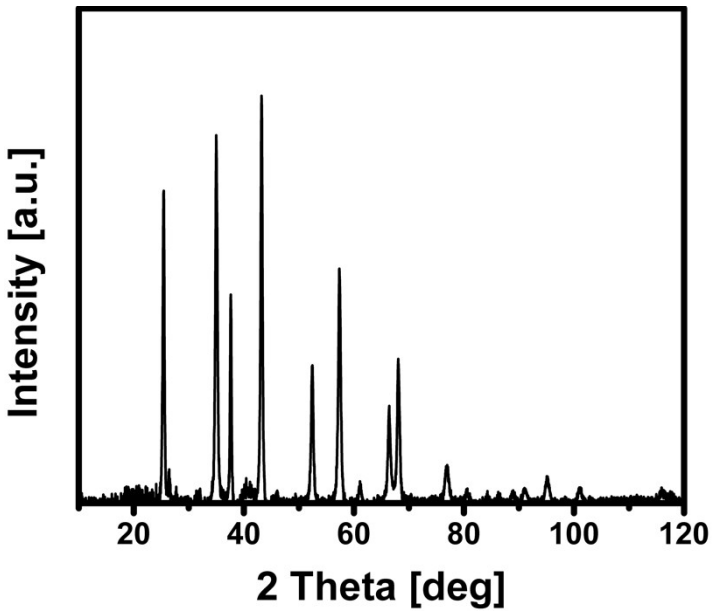

Fig. S11: XRD of tris[(diethyl-2-nitromalonato)]aluminum(III) annealed at 800 °C.

Tab.S2: Summary of XRR and specroscopic ellipsometry measurements.

method	sample	thickness (nm)	density (g/cm^3)
XRR	**Al_xO_y-200**	170	2,18
ellipsometry	**Al_xO_y-200**	169,55	/
XRR	**Al_xO_y-350**	122	2,26
ellipsometry	**Al_xO_y-350**	123,89	/

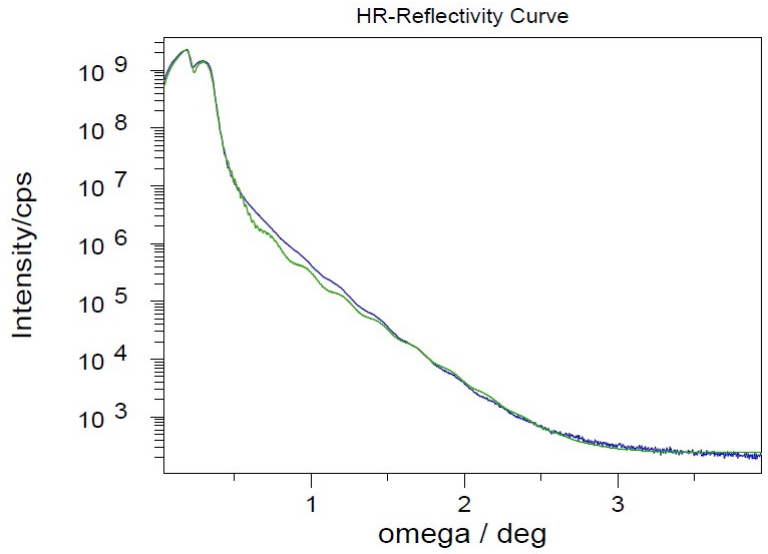

Fig. S12: XRR measurement of Al_xO_y-200.

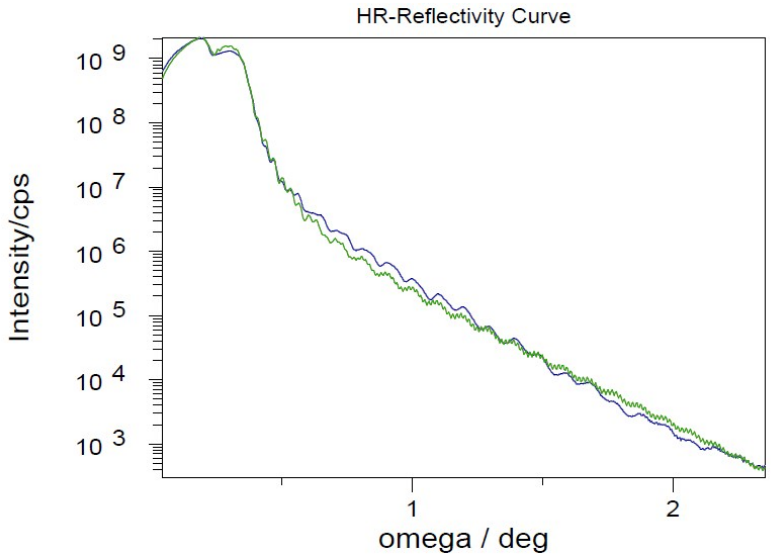

Fig. S13: XRR measurement of Al_xO_y-350.

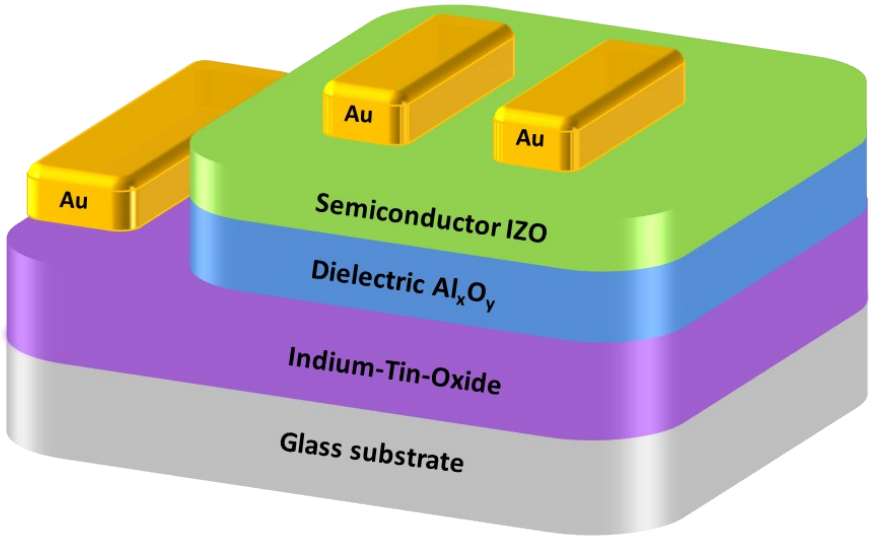

Fig. S14: Schematic representation of the device geometry of the fabricated thin film transistor.