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

Water adsorption at zirconia: From the $ZrO_2(111)/Pt_3Zr(0001)$ model system to powder samples

Peter Lackner, Jan Hulva, Eva-Maria Köck, Wernfried Mayr-Schmölzer, Joong Il J. Choi, Simon Penner, Ulrike Diebold, Florian Mittendorfer, Josef Redinger, Bernhard Klötzer, Gareth S. Parkinson, and Michael Schmid

Supporting Information

1 Summary of procedures

Preparation step	Step	Temperature	Gas, (Pressure)	Time (min)
Cleaning Pt_3Zr	Sputtering	RT	Ar or Ne	20
	Last sputter cycle before oxidation	Linear ramp 680 K to 300 K	Ar or Ne	20
	Annealing	1175 K	-	
Oxide preparation	Oxidation	680 K	O_2, 10^{-7} mbar	10
	Annealing	RT-STM: ≈1205 K TPD, XPS: 1205 K LT-STM: 1160 K	-	30
D_2O TPD		100 K to 550 K 1 or 2 K/s (see figure caption)		
CO_2 TPD		50 K to 300 K 1 K/s		

Table S1: Overview of the preparation procedures and TPD temperature ramps used in the current work.

2 Overview STM Images of ZrO_2/Pt_3Zr Films

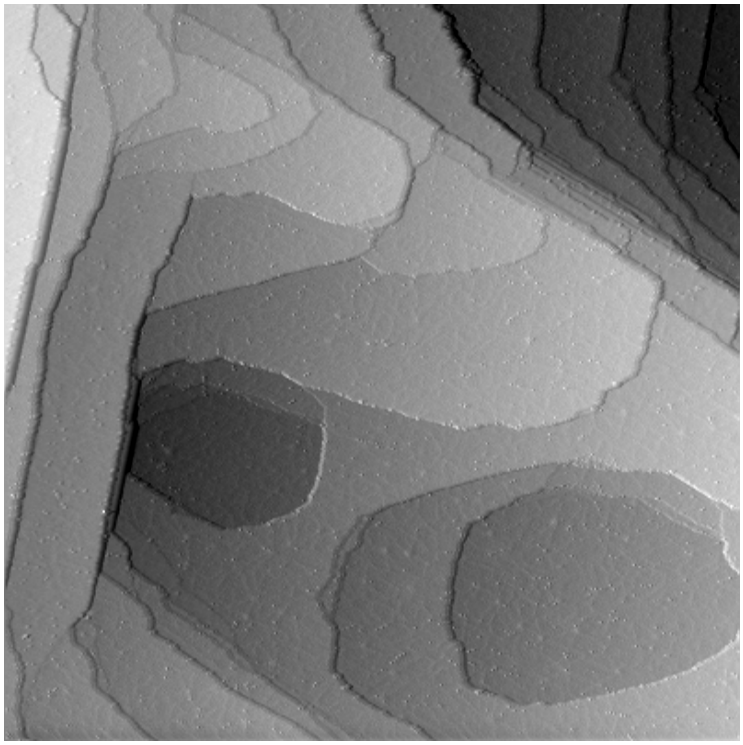

Figure S1: Overview STM image (200×200 nm^2, −0.1 V, 0.1 nA, 78 K) of the $ZrO_2/Pt_3Zr(0001)$ surface prepared in the LT-STM system. For improved contrast, the image is displayed as if illuminated from the left.

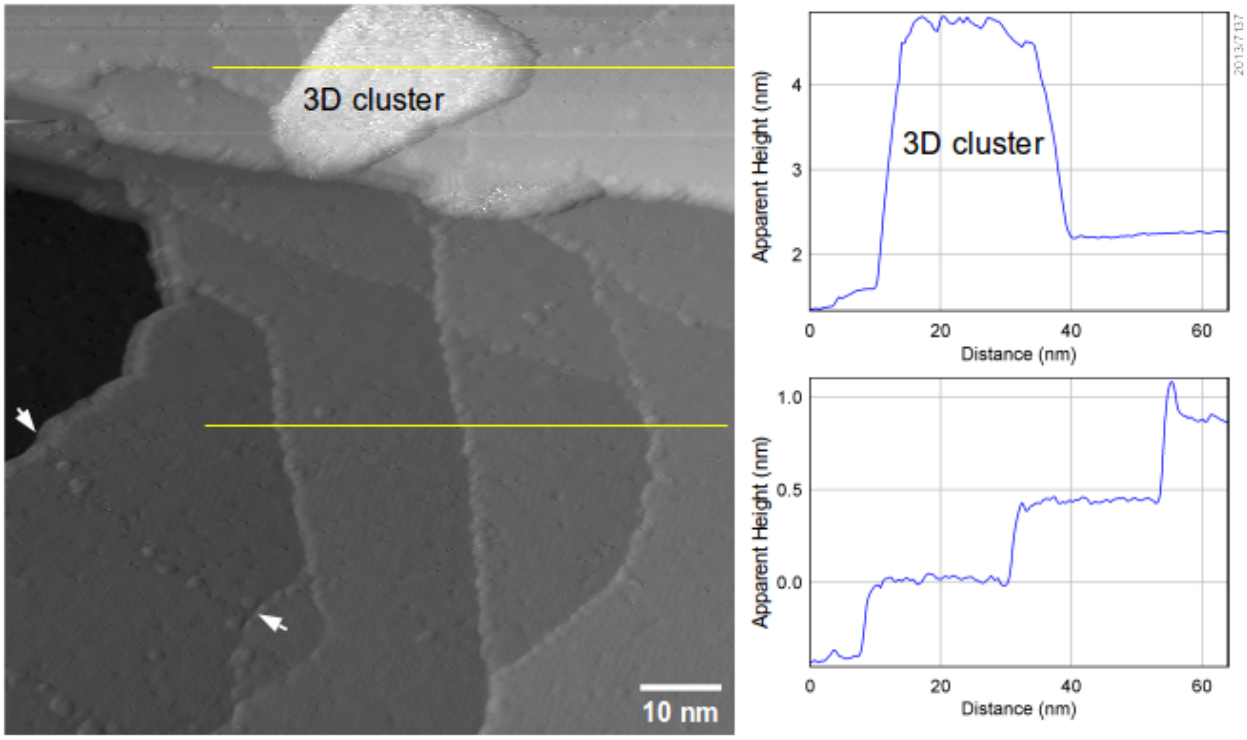

Figure S2: Overview STM image (4.1 V, 0.1 nA, room temperature) of the $ZrO_2/Pt_3Zr(0001)$ oxide annealed at 1200 K with a 3D oxide cluster. For improved contrast, the image is displayed as if illuminated from the left. Line scans along the yellow lines are shown at the right; the bottom one shows the 0.4 nm steps of the substrate between equivalent terminations (a few steps of 0.2 nm height are seen with weaker contrast in other parts of the image). Two white arrows indicate the ends of an orientational domain boundary of the trilayer oxide. The noisy appearance of the cluster surface and the tip changes (horizontal streaks) when imaging the 3D cluster are due to its insulating nature.