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SUPPORTING INFORMATION FOR:

Structure and Reactivity of a Model Oxide Supported Silver Nanocluster Catalyst Studied by Near Ambient Pressure X-ray Photoelectron Spectroscopy

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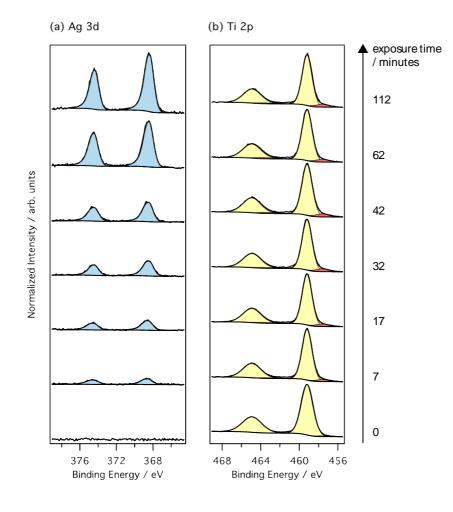
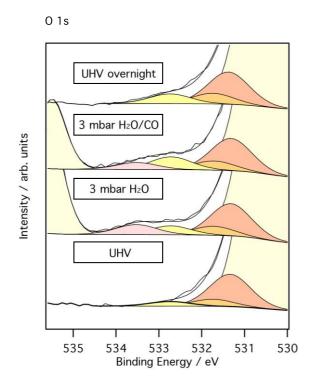


Figure S1. Core level photoelectron spectra for (a) Ag 3d and (b) Ti 2p

Complete set of Ag 3d XPS core-level spectra (a) with the corresponding Ti 2p corelevel spectra (b) (hv = 1 keV) showing, from bottom to top, an increasing Ag coverage. The spectra are normalized to the intensity of the Ti 2p Ti⁴⁺_{3/2} peak at 459.2 eV.

Figure S2. Enlarged Core level NAP-XPS spectra for O 1s showing components due

to H2O and CO exposure in more detail.



O 1s core- level NAP-XPS spectra recorded at UHV, under exposure to 3 mbar H_2O , under exposure to 3mbar H_2O/CO and at UHV the following day. The O 1s spectra highlight the high binding energy shoulder shown in Figure 4 of the main manuscript for clarity.

The assignment of the fitted peaks for the O 1s, Ti 2p and Ag 3d is given below in Table S1. The gas phase O 1s peaks are not included in the table. These occur at 535.5 eV (H₂O) and 538.2 eV (CO).

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Table S1. Binding energy and assignment of Ti 2p, O 1s and Ag 3d XPS core-level

peaks.

	UHV		3 mbar H ₂ O		3 mbar		UHV-next day	
					H₂O/CO			
Assignment	BE /	%	BE \	%	BE / eV	%	BE \ eV	%
	eV	±1%	eV	±1 %	± 0.1 eV	±1 %	± 0.1 eV	±1 %
	± 0.1		± 0.1					
	eV		eV					
Ti ³⁺	457.7	7.3	457.7	6.3	457.7	6.7	457.7	5.2
TI ⁴⁺	459.2	92.7	459.2	93.7	459.2	93.3	459.2	94.8
TI <u>O</u> 2	530.4	88.0	530.4	84.3	530.4	84.1	530.4	86.2
O intrinsic ¹	531.4	8.8	531.3	8.4	531.3	8.4	531.3	8.6
Odefect/OHads	531.8	1.9	531.7	2.3	531.7	2.4	531.7	2.6
Odefect/COads/OHads	532.7	1.2	532.7	2.0	532.7	3.3	532.7	2.1
H ₂ O	-	0	533.5	2.6	533.5	1.8	-	0
Ag ^{δ+/} Ag(III)	-	0	-	-	367.6	5.5	367.6	0
Ag(0)	368.4	100	368.4	100	368.4	89.0	368.4	100
Ag(III) _{satellite}	-	0	-	0	371.4	5.5	371.4	0
	Ti ³⁺ TI ⁴⁺ TIO2 Ointrinsic ¹ Odefect/OHads Odefect/OHads H2O H2O Ag ^{δ+/} Ag(III) Ag(0)	AssignmentBE /AssignmentBE /eV± 0.1± 0.1eVTl ³⁺ 457.7Tl ⁴⁺ 459.2Tl02530.4Ointrinsic ¹ 531.4Odefect/OHads531.8Odefect/COads/OHads532.7H2O-Ag ^{δ+/} Ag(III)-Ag(0)368.4	Assignment BE / % eV ±1% ±0.1 ±1% t0.1 2 rl³+ 457.7 7.3 TlQ2 530.4 88.0 Ointrinsic ¹ 531.4 8.8 Odefect/OHads 531.8 1.9 H2O - 0 Ag ^{5+/} Ag(III) - 0 Ag(0) 368.4 100	AssignmentBE /%BE \AssignmentBE /%BE \eV±1%eV±0.1±0.1±0.1±0.1eVft ³⁺ 457.77.3457.7TI ⁴⁺ 459.292.7459.2TIQ2530.488.0530.4Olintrinsic ¹ 531.48.8531.3Odefect/OHads531.81.9531.7H2O-0533.5Ag ^{5+/} Ag(III)-0568.4Ag(0)368.4100368.4	AssignmentBE /%BE \%eV±1%eV±1%±0.1±0.1±0.1±0.1±0.140.110eVrl³+457.77.3457.76.3Tl⁴+530.488.0530.484.3Ointrinsic1531.48.8531.38.4Odefect/OHads531.71.2531.72.3H2O-532.71.2533.52.6Ag⁵+/Ag(III)-0538.4100368.4100	AssignmentBE /%BE \H₂ O/COAssignmentBE /%BE \BE /%eV11%eV11%10.1 eV± 0.1± 0.1± 0.1± 0.1 eV10.1 eVt ³ 45.11eV110.1 eVTi ³⁺ 457.77.3457.76.3457.7Tl ⁴⁺ 459.292.7459.293.7459.2Tl ⁰ 2530.488.0530.484.3530.4Ontrinsic ¹ 531.48.8531.38.4531.3Odefect/OHads531.71.2532.72.3532.7H2O-1.2533.52.6533.5Ag(0)368.4100368.4100368.4	AssignmentBE /%BE \%BE / eV%eV±1%eV±1%±0.1 eV±0.1 eV±1%±0.1±0.1±0.1±0.1 eV±0.1 eV±0.1 eVeV±0.1±0.1±0.11/21/2T ³⁺ 457.77.3457.76.3457.76.3Tl ⁴⁺ 459.292.7459.293.7459.293.3TlQ2530.488.0530.484.3530.484.1Olefter/OHads531.81.9531.72.3531.72.4Ag69/536.4100533.52.653.53.63.6	AssignmentBE /%BE / eV%BE / eV%BE / eVeV±1%eV±1%±1.4±0.1 eV±0.1 eV±0.1 eV±0.1±0.1±0.1±0.1±0.1±0.1 eV±0.1 eVeV±0.1±0.1±0.1111eV±0.1£0.11111rl³-457.77.3457.76.3457.76.7459.2Tl⁴-530.4530.7530.4530.4530.4530.4530.4flog531.4531.3531.7531.3531.7531.3531.7Oderect/OHads531.81.2532.72.0532.73.3532.7flog11.2532.72.0532.51.852.7flog53.41.2533.52.653.51.852.7flog53.41.053.52.653.51.852.7flog53.41.053.52.653.51.852.7flog53.41.053.52.653.51.852.7flog53.41.053.52.653.55.553.6flog53.453.55.553.55.553.453.4flog53.553.553.553.553.553.553.5flog53.553.553.553.553.553.553.5flog53.553.5

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