

# Central Lancashire Online Knowledge (CLoK)

Title	Structure and Reactivity of a Model Oxide Supported Silver Nanocluster Catalyst Studied by Near Ambient Pressure X-ray Photoelectron Spectroscopy
Туре	Article
URL	https://clok.uclan.ac.uk/id/eprint/19909/
DOI	https://doi.org/10.1021/acs.jpcc.7b05818
Date	2017
Citation	Wagstaffe, Michael, Hussain, Hadeel, Acres, Matthew, Jones, Rosemary, Syres, Karen orcid iconORCID: 0000-0001-7439-475X and Thomas, Andrew G. (2017) Structure and Reactivity of a Model Oxide Supported Silver Nanocluster Catalyst Studied by Near Ambient Pressure X-ray Photoelectron Spectroscopy. The Journal of Physical Chemistry C, 121 (39). pp. 21383- 21389. ISSN 1932-7447
Creators	Wagstaffe, Michael, Hussain, Hadeel, Acres, Matthew, Jones, Rosemary, Syres, Karen and Thomas, Andrew G.

It is advisable to refer to the publisher's version if you intend to cite from the work. https://doi.org/10.1021/acs.jpcc.7b05818

For information about Research at UCLan please go to <a href="http://www.uclan.ac.uk/research/">http://www.uclan.ac.uk/research/</a>

All outputs in CLoK are protected by Intellectual Property Rights law, including Copyright law. Copyright, IPR and Moral Rights for the works on this site are retained by the individual authors and/or other copyright owners. Terms and conditions for use of this material are defined in the <u>http://clok.uclan.ac.uk/policies/</u>

## SUPPORTING INFORMATION FOR:

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

Michael Wagstaffe,<sup>†</sup> Hadeel Hussain,<sup>‡</sup><sup>@</sup> Matthew Acres,<sup>‡</sup> Rosemary Jones,<sup>§</sup> Karen

L. Syres,  $*^{\P}$  and Andrew G. Thomas  $^{* \ddagger \$}$ 

<sup>†</sup> School of Physics and Astronomy, The University of Manchester, Oxford Road, M13 9PL, UK.

<sup>‡</sup> School of Materials, The Mill, The University of Manchester, Sackville Street, Manchester, M13 9PL, UK.

\$ Photon Science Institute, The University of Manchester, Oxford Road, Manchester, M13 9PL, UK .

<sup>¶</sup>Jeremiah Horrocks Institute, The University of Central Lancashire, Fylde Road, Preston, PR1 2HE, UK.

@Current address: Diamond Light Source, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0DE, UK.

#### E-mail: andrew.g.thomas@manchester.ac.uk



### 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 Ti<sup>4+</sup><sub>3/2</sub> 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 (H<sub>2</sub>O) and 538.2 eV (CO).

S 3

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

peaks.

		UHV		3 mbar H <sub>2</sub> O		3 mbar		UHV-next day	
						H₂O/CO			
Species	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 2p <sub>3/2</sub>	Ti <sup>3+</sup>	457.7	7.3	457.7	6.3	457.7	6.7	457.7	5.2
	TI <sup>4+</sup>	459.2	92.7	459.2	93.7	459.2	93.3	459.2	94.8
0 15	TI <u>O</u> 2	530.4	88.0	530.4	84.3	530.4	84.1	530.4	86.2
	<b>O</b> intrinsic <sup>1</sup>	531.4	8.8	531.3	8.4	531.3	8.4	531.3	8.6
	Odefect/OH <sub>ads</sub>	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 <sub>2</sub> O	-	0	533.5	2.6	533.5	1.8	-	0
Ag 3d <sub>5/2</sub>	Ag <sup>δ+/</sup> 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) <sub>satellite</sub>	-	0	-	0	371.4	5.5	371.4	0

 Jackman, M. J.; Thomas, A. G.; Muryn, C. Photoelectron Spectroscopy Study of Stoichiometric and Reduced Anatase TiO<sub>2</sub>(101) Surfaces: The Effect of Subsurface Defects on Water Adsorption at Near-Ambient Pressures. J. Phys. Chem. C 2015, 119, 13682–13690.