

Near ambient pressure XPS study of Au oxidation.

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SUPPORTING INFORMATION.

Table S1:

	bulk		surface		restructuring		oxide	
	BE	FWHM	BE	FWHM	BE	FWHM	BE	FWHM
	(eV)	(eV)	(eV)	(eV)	(eV)	(eV)	(eV)	(eV)
Before O ₃	83.92	0.486	83.60	0.415	-	-	-	-
During O ₃	83.92	0.486	83.59	0.415	83.29	0.499	85.22	1.105
After O ₃	83.92	0.486	83.60	0.415	83.29	0.500	-	-

Depth profile quantification

The gold oxide thickness can be estimated by quantification of depth profile. For calculation we use the equation for semi-infinite specimen, with uniform over-layer of thickness t_A ³⁰. Suffixes S (support, Au⁰) and A (active over-layer, Au^{δ+}) are used to specify the nature of the atomic species. Over-layer/substrate ratio:

$$\frac{N_A}{N_S} = \frac{F_A r_A s_A / \lambda_{Aa}}{F_S r_S s_S / \lambda_{Sa}} \cdot \frac{[1 - \exp(-t_A / \lambda_{Aa} \sin \vartheta)]}{\exp(-t_A / \lambda_{Sa} \sin \vartheta)}, \quad (S1)$$

where F , dependent on the emitted electron energy, includes several instrumental parameters; ρ , the atomic density; σ , the differential cross-section; λ , IMPF; where θ is the emission direction

angle with respect to the surface normal.. Equation S1 applies to several situations, including growth on metal³¹.

In our calculation we use the following parameters: $F_{Au^0} = F_{Au^{+\delta}}$; $\lambda_{Au^0} = \lambda_{Au^{+\delta}}$; $\sigma_{Au^0} = \sigma_{Au^{+\delta}}$; $\rho_{Au^0} = 5.9 * 10^{22}$ atom/mol; $\rho_{Au^{+\delta}} = 3.09 * 10^{22}$ atom/mol ; $\theta = 90^\circ$, that leads to the Au oxide thickness of 0.29 nm.