

Supporting Information

Geometric and electronic structure of Au on Au/CeO₂ catalysts during the CO oxidation: Deactivation by reaction induced particle growth

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Table S1

EXAFS structural parameters of Au NPs on the CeO₂ support during CO oxidation reaction at 80°C (1% CO, 1% O₂, 98% N₂) after different pre-treatments (O400 and CO400) and after different reaction time intervals (data fit in k -range of 3.0 - 9.3 Å⁻¹ and R-range of 0.5 - 4.8 Å).

CN: coordination number, DW: Debye-Waller factor, r: distance, E₀: energy shift.

Time / min	Scatterer	CN	DW / 10 ⁻³ Å ²	r / Å	E ₀ / eV	Dispersion / % (*)
O400 / 0	Au-Au / Au-O	6.3 / 0.5	9.74 / 1.0	2.84 / 1.96	0.65 / 19.7	54.0
O400 / 61	Au-Au	7.6	13.0	2.84	-1.0	34.0
O400 / 175	Au-Au	8.0	14.5	2.85	-1.00	32.0
O400 / 290	Au-Au	7.9	14.4	2.83	-0.27	37.0
CO400 / 0	Au-Au	4.1	12.0	2.80	-1.7	100
CO400 /	Au-Au	4.2	8.5	2.80	-0.84	100
CO400 /	Au-Au	5.9	10.8	2.77	2.4	60

(*) calculated from CN according to data for supported Au NPs in Miller et al. [1].

Figure S1 XANE spectra of the Au/CeO₂ catalyst directly after CO400 pre-treatment (10% CO/N₂, 30 min at 400°C; red line) at 80°C in N₂ and during the CO oxidation reaction at 80°C (1% CO, 1% O₂, 98% N₂) after different reaction times (2, 30, and 178 min, blue lines). The spectrum recorded from a Au foil is presented for comparison (black line, bottom).

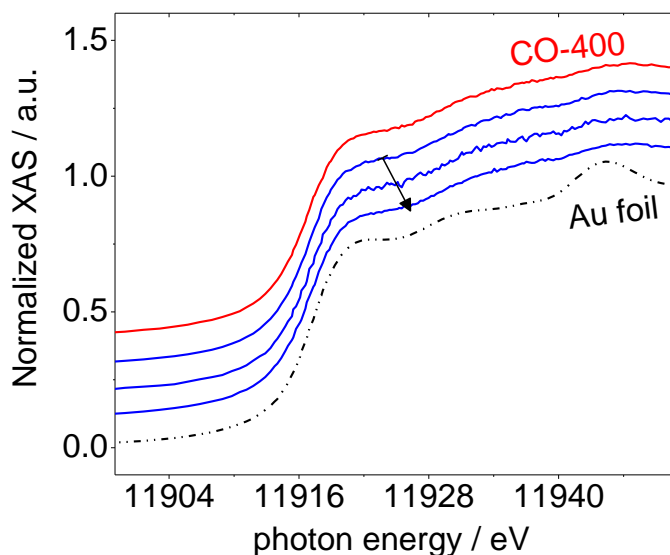
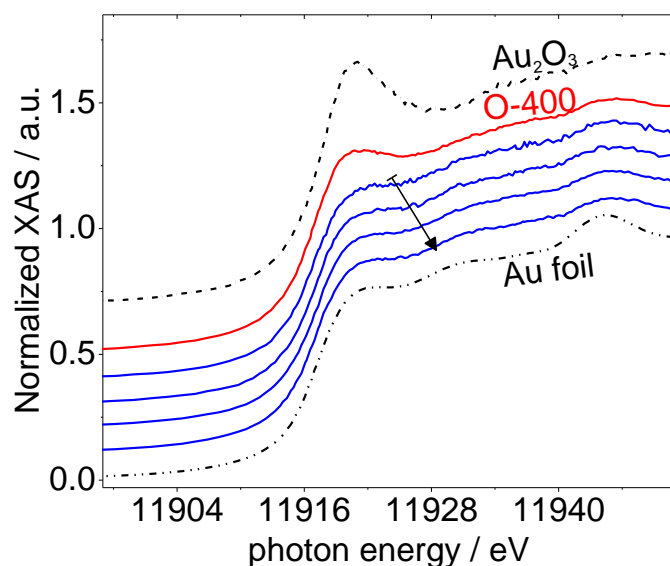


Figure S2 XANE spectra of the Au/CeO₂ catalyst directly after O400 pre-treatment (10% O₂/N₂, 30 min at 400°C; red line) at 80°C in N₂ and during the CO oxidation reaction at 80°C (1% CO, 1% O₂, 98% N₂) at different reaction times (2, 23, 61, 174 min, blue lines). The spectra of Au₂O₃ (black line, top) and Au foil (black line, bottom) are presented for comparison.



References

- [1]. Miller, J T, Kropf, A J, Zha, Y, Regalbuto, J R, Delannoy, L, Louis, C, Bus, E and van Bokhoven, J A 2006 *J.Catal.* **240** 222-234.