Electronic Supplementary Information for

Modifications of the metal and support during the deactivation and regeneration of Au/C catalysts for the hydrochlorination of acetylene

Marco Conte,*[a] Catherine J. Davies,[a] David J. Morgan,[a] Thomas E. Davies,[a] Albert F. Carley,[a] Peter Johnston,[b] and Graham J. Hutchings *[a]

[a] Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Cardiff, CF10 3AT, UK

[b] Johnson Matthey Catalysts, Orchard Road, Royston, Herts, SG8 5HE, UK

*E-mail: ConteM1@cardiff.ac.uk, Hutch@cardiff.ac.uk

Table of contents:

Fig. S15. XPS spectrum and simulation for Au/C catalyst after third re-oxidation.

Fig. S16. N_2 adsorption isotherms for the untreated carbon, fresh Au/C catalyst and oxidised Au/C catalyst.

Fig. S17. Pore size distribution of the untreated carbon, fresh Au/C catalyst and oxidised Au/C catalyst.

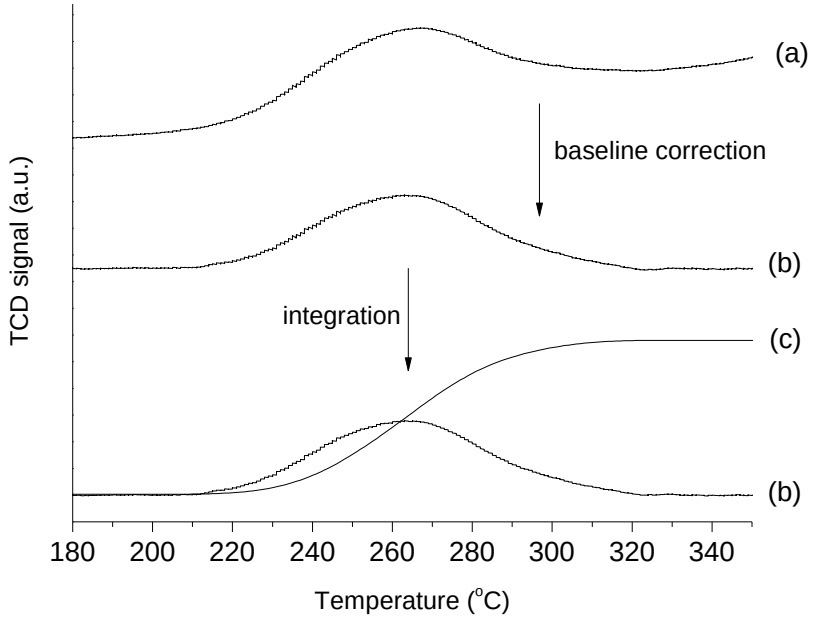


Fig. S1. Procedure for the TPR area peaks determination. The Au^{3+} peak (a) was subject to baseline correction (b). A cumulative area counts in the interval 180 to 350 ^{o}C (c) was carried out.

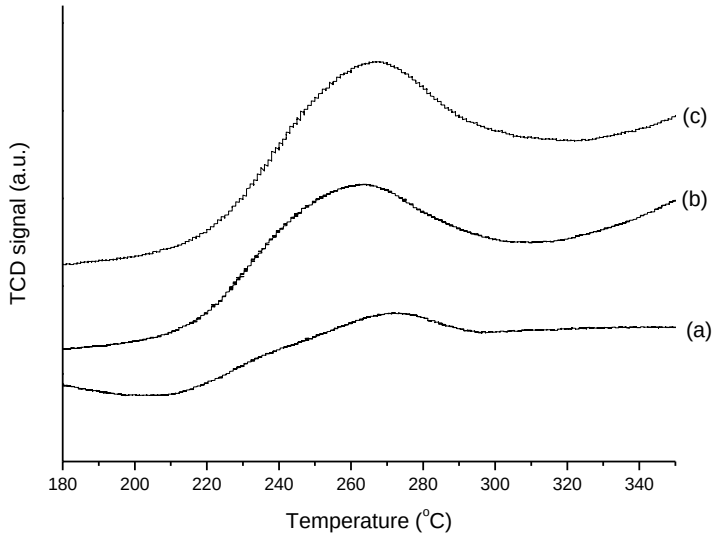
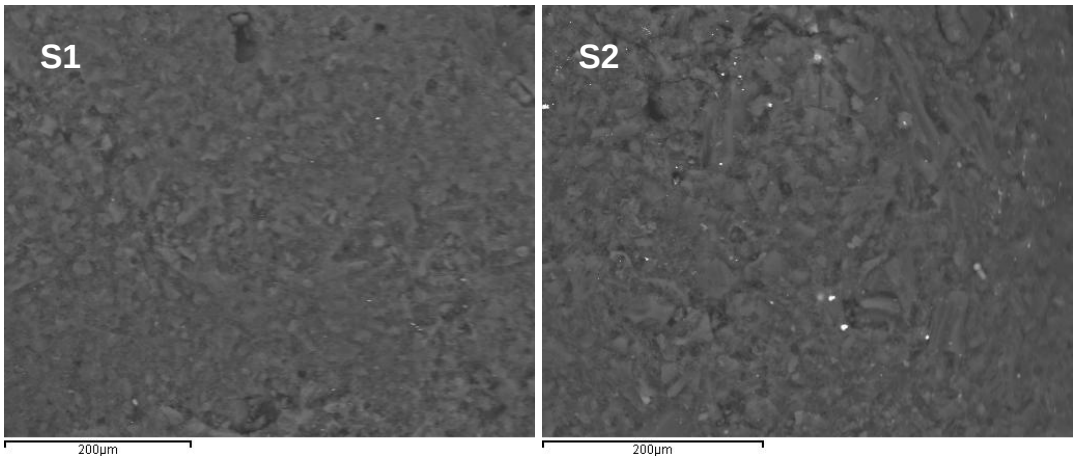


Fig. S2. Details of the TPR thermograms in the region 180-350 °C (Au^{3+} reduction). (a) fresh catalyst, (b) first catalyst oxidation, and (c) second catalyst oxidation.



Figs. S3 and S4. SEM images of the Au/C catalyst 1% wt.

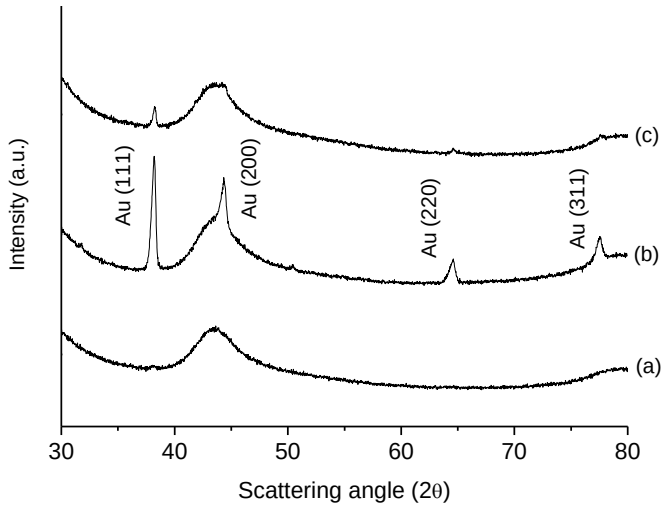


Fig. S5. XRPD patterns of the Au/C catalyst 1% wt impregnated in *aqua regia* dried at (a) 110 ^{o}C, (b) 140 ^{o}C and (c) 180 ^{o}C.

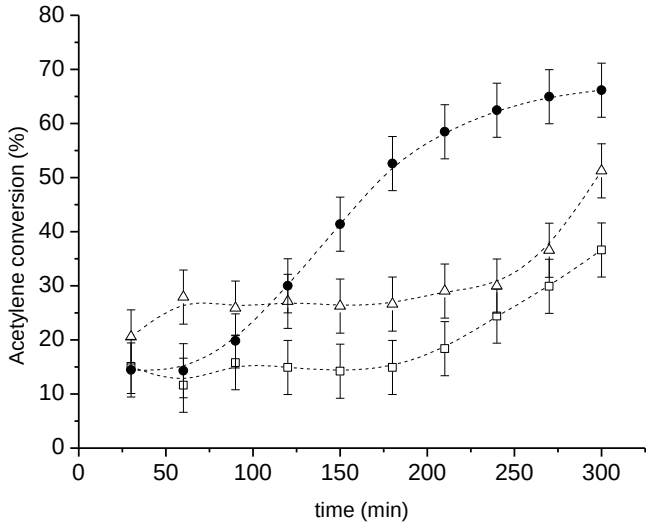


Fig. S6. Acetylene conversion by using catalysts impregnated in *aqua regia* drying the catalysts at different temperatures of: (□) 110, (●) 140 and (Δ) 180 ^{o}C.

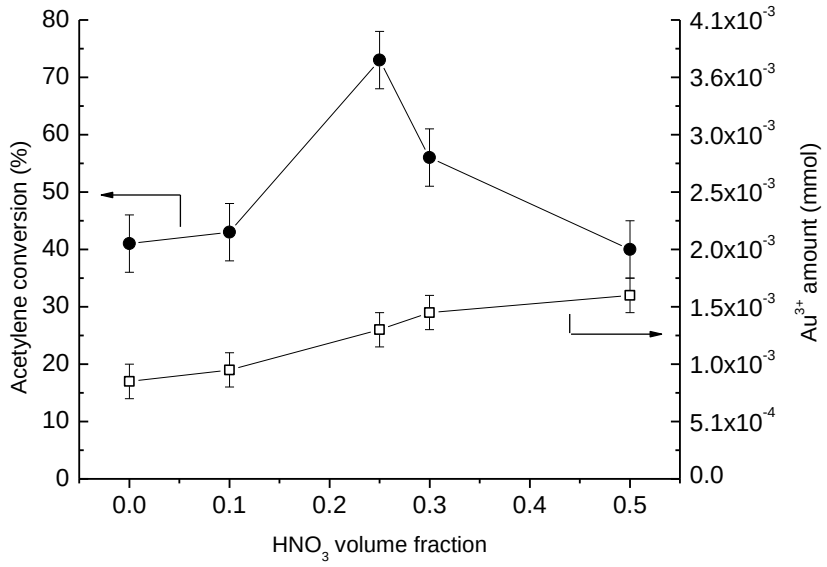


Fig. S7. Conversion (●) after 5 h and Au^{3+} (□) amount (in mmol) for Au/C catalysts containing different amount of Au^{3+}. The catalysts were obtained from impregnating solutions containing different HNO_3 volume fraction in the HCl/HNO_3 mixture.

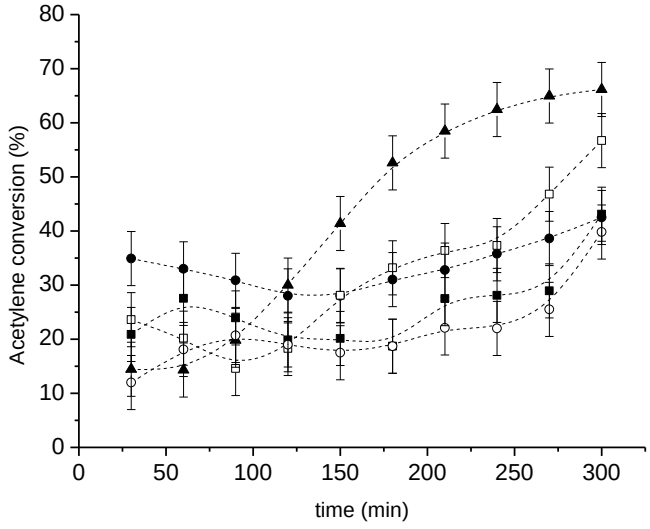


Fig. S8. Acetylene conversion over Au/C catalysts dried at 140 ^{o}C using different HNO_3 volume fraction in the HCl/HNO_3 preparation mixture: (■) 0, (●) 0.1, (▲) 0.25, (□) 0.33 and (○) 0.5 HNO_3 volume fraction.

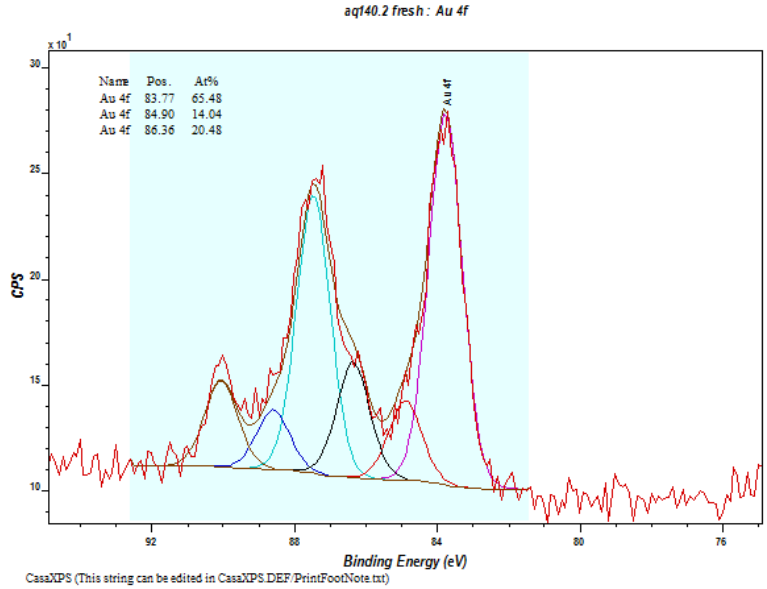


Fig. S9. XPS spectrum and simulation for a fresh Au/C catalyst.

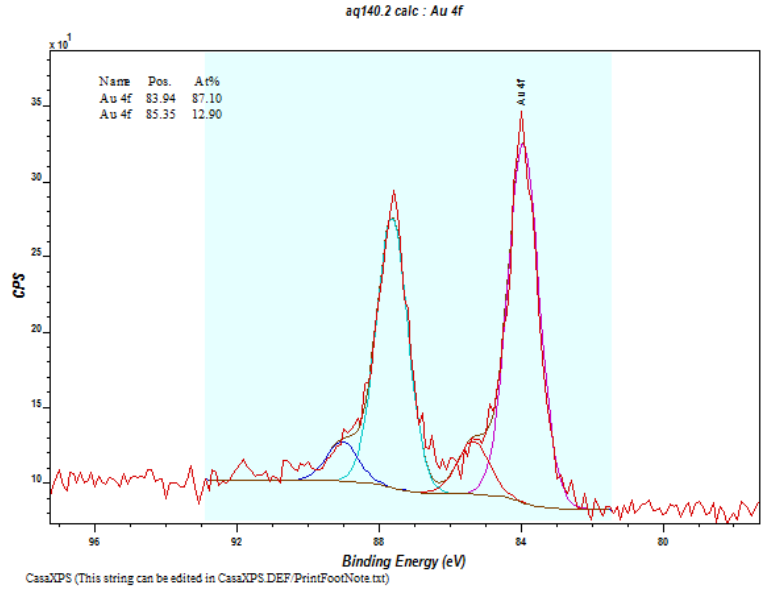


Fig. S10. XPS spectrum and simulation for a reduced Au/C catalyst.

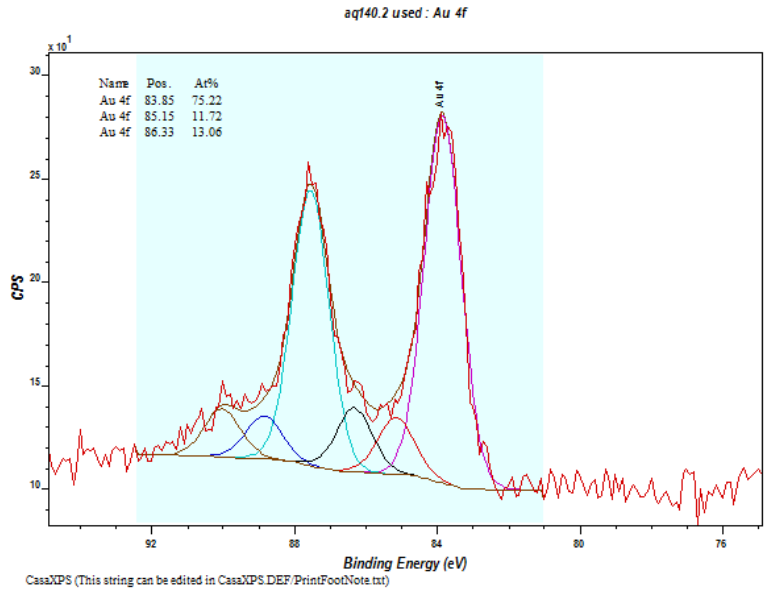


Fig. S11. XPS spectrum and simulation for Au/C catalyst after first re-oxidation.

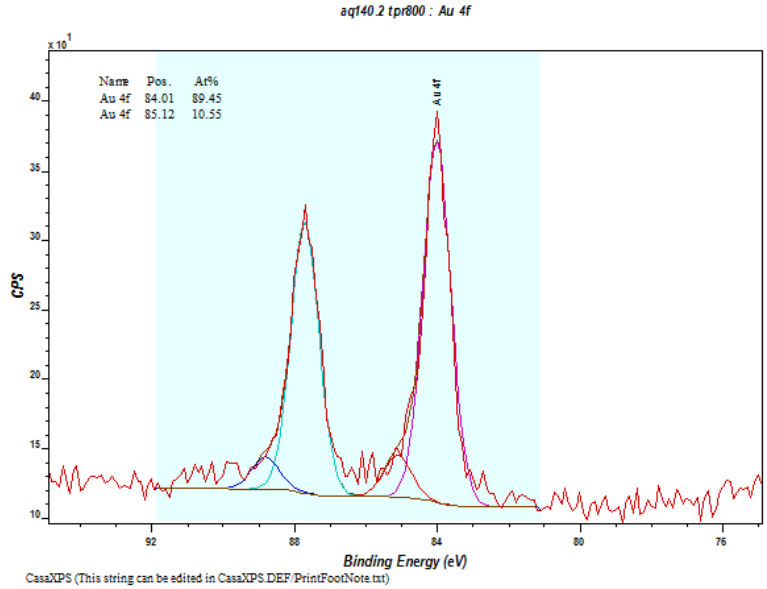


Fig. S12. XPS spectrum and simulation for Au/C catalyst after second reduction.

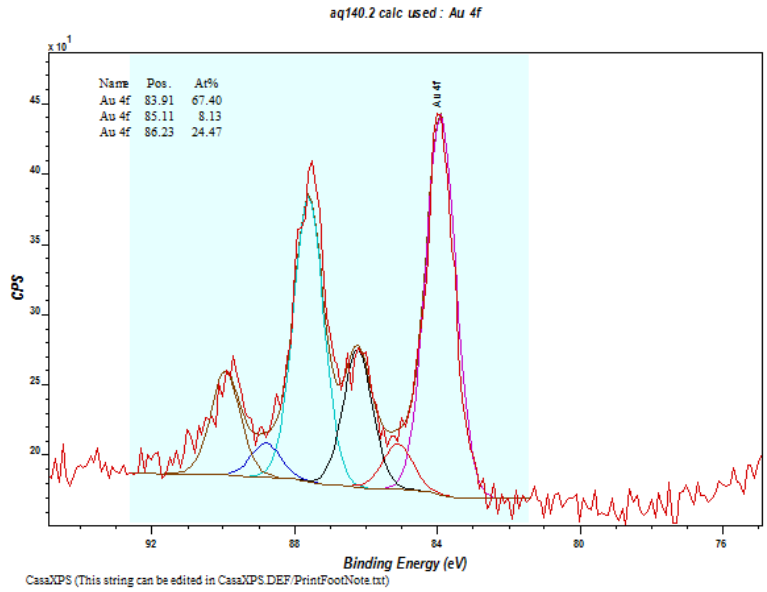


Fig. S13. XPS spectrum and simulation for Au/C catalyst after second re-oxidation.

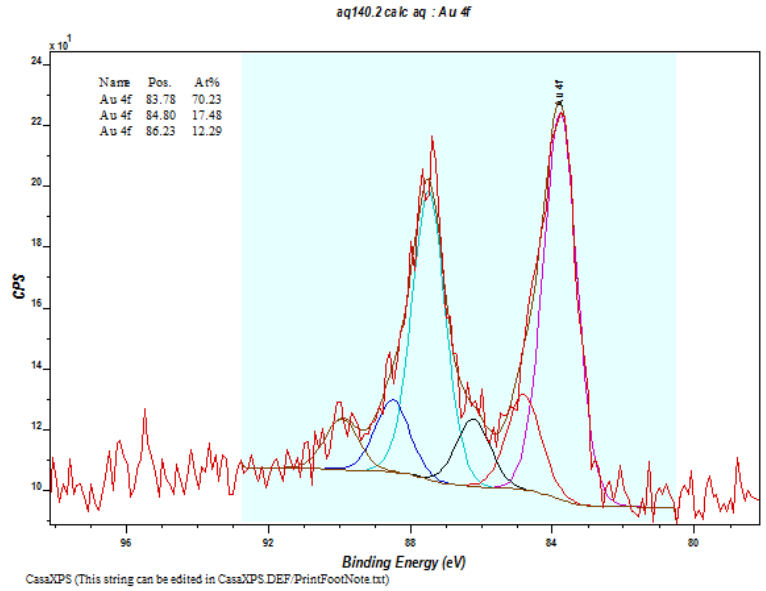


Fig. S14. XPS spectrum and simulation for Au/C catalyst after third reduction.

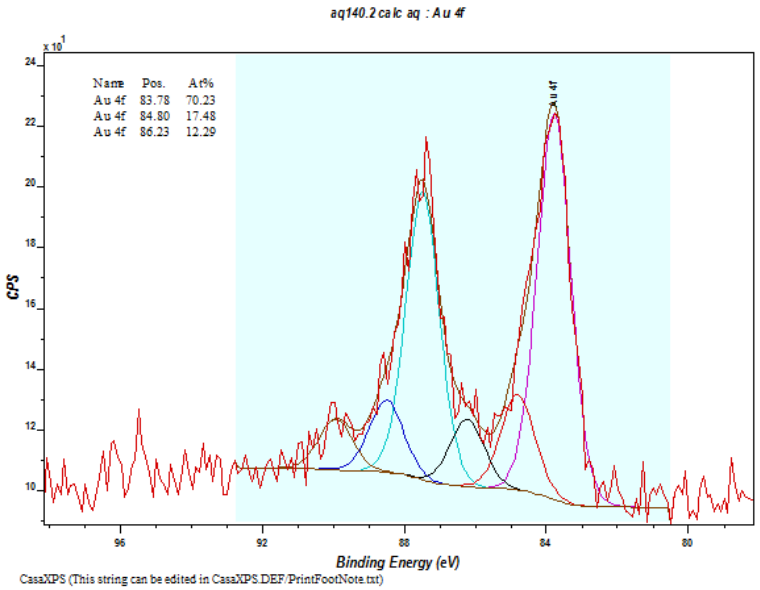


Fig. S15. XPS spectrum and simulation for Au/C catalyst after third re-oxidation

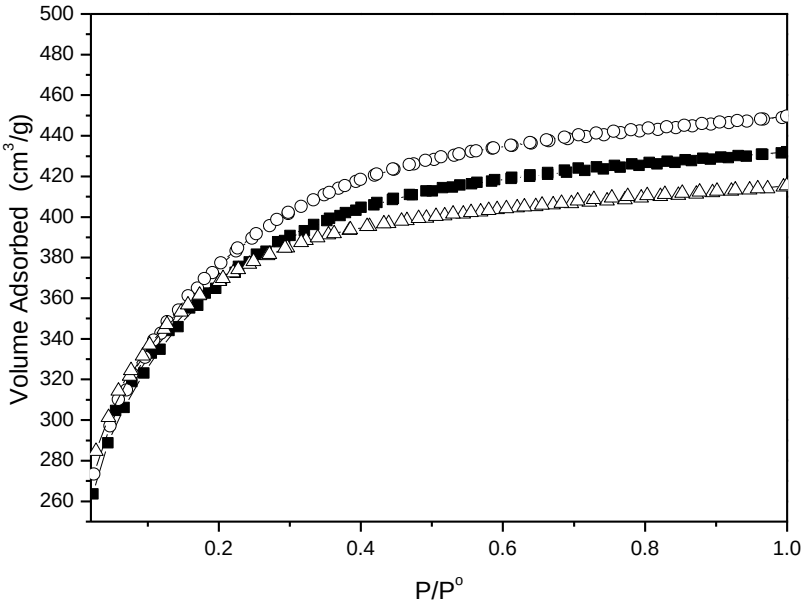


Fig. S16. N_2 adsorption isotherms measured at 77K. (Δ) untreated carbon (Norit ROX 0.8), (■) fresh Au/C catalyst and (○) Oxidised Au/C catalyst.

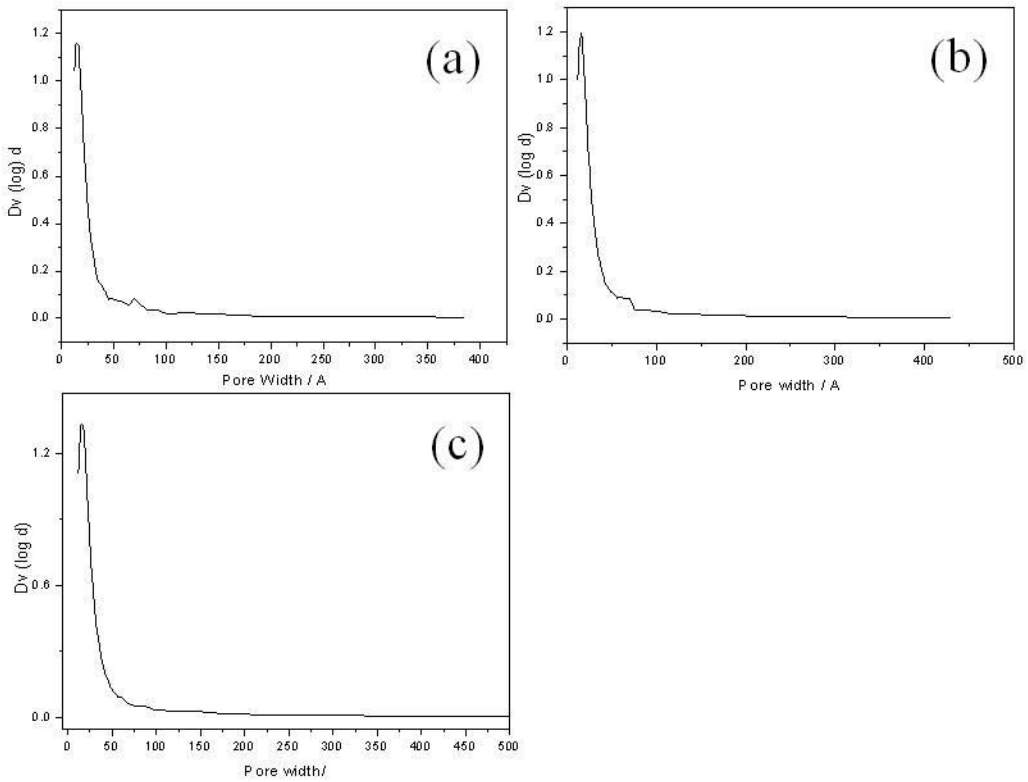


Fig. S17. Pore size distribution of (a) untreated carbon (Norit ROX 0.8), (b) fresh Au/C catalyst and (c) Oxidised Au/C catalyst.

Table S1 Quantification (in mmol) and identification from XPS of Au species over Au/C catalysts subejct to reduction and oxidation cycles.

Catalyst treatment	**Au species (mmol)**			**Binding energies (eV)**		
	Au^{3+}	**Au^{0}**	**Au^{0}-s**	**Au^{3+}**	**Au^{0}**	**Au^{0}-s**
fresh catalyst	1.04E-03	3.33E-03	7.11E-04	86.4	83.8	84.9
1^{st} reduction	0.00E+00	4.42E-03	6.55E-04	-	83.9	85.4
1^{st} oxidation	6.65E-04	3.82E-03	5.94E-04	86.3	83.9	85.2
2^{nd} reduction	0.00E+00	4.54E-03	5.38E-04	-	84	85.1
2^{nd} oxidation	1.24E-03	3.42E-03	4.11E-04	86.2	83.9	85.1
3^{rd} reduction	0.00E+00	4.57E-03	5.08E-04	-	84	85.3
3^{rd} oxidation	6.24E-04	3.56E-03	8.88E-04	86.2	83.8	84.8