Supporting Information

Characterization of Surface Structure and Oxidation/Reduction Behaviour of $Pd-Pt/Al_2O_3$ Model Catalysts

Natalia M. Martin,*,† Johan Nilsson,† Magnus Skoglundh,† Emma C. Adams,†

Xueting Wang,† Peter Velin,† Gudmund Smedler,‡ Agnes Raj,¶ David

Thompsett,¶ Hidde H. Brongersma,§ Thomas Grehl,∥ Giovanni Agostini,¹ Olivier

Mathon,¹ Stefan Carlson,# Katarina Norén,# Francisco J. Martinez-Casado,#

Zdenek Matej,# Olivier Balmes,# and Per-Anders Carlsson†

Competence Centre for Catalysis, Chalmers University of Technology, Gothenburgh, 412
96, Sweden, Johnson Matthey AB, Västra Frölunda, 421 31, Sweden, Johnson Matthey
Technology Centre, Blounts Court, Sonning Common, Reading, RG4 9NH, UK,

Department of Applied Physics, Eindhoven University of Technology, Eindhoven, 5600, The
Netherlands, ION-TOF GmbH, Münster, Germany, European Synchrotron Radiation
Facility, Grenoble, 38043, France, and MAX-IV Laboratory, Lund University, Lund, 221
00, Sweden

E-mail: Natalia.Martin@chalmers.se

Phone: +46 (0)31-772 29 04.

Figure S1 displays the Pd K edge EXAFS spectra after the PdPt samples have been reduced in 2% H₂ (a) or oxidised in 1.5 % O₂ (b). The EXAFS analysis indicates that, during oxidation, the Pd atoms are in an oxidised state similar to PdO, but when they are in a reduced state the PdO phase is reduced to a state which is closer to metallic Pd. No contribution from Pd-metal scattering at oxidising conditions could be observed indicating that Pd is fully oxidised.

Figures S2 and S3 show the evolution of the XAFS spectra for the Pd-Pt F800 and L800 samples at 360 °C during the oxidation-reduction cycling experiment in either 1.5 % O_2 or 2 % H_2 . The experiment starts with a 5 min oxidation pulse. The left panel (a) shows XAS spectra recorded at the end of the oxidation and reduction periods, while the right panel shows the recorded XAS spectra as a function of time (b) together with the white line intensity during the experiment (c).

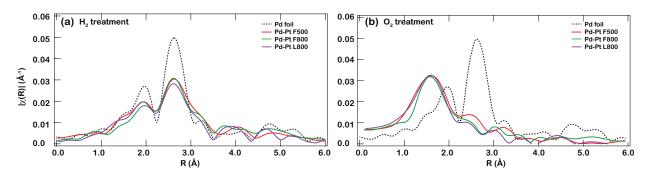


Figure S1: Magnitude of Fourier Transformed Pd K edge EXAFS spectra recorded in situ from the reduced (a) and oxidized (b) Pd-Pt/Al₂O₃ catalysts at 360 °C (k-weight = 0). Pd foil is included as a reference. The spectra are taken during the transient oxidation/reduction measurement as shown in Figure 6 with a time resolution of 0.5 sec, therefore the poor data quality.

^{*}To whom correspondence should be addressed

[†]Chalmers University

[‡]Johnson Matthey, Sweden

[¶]Johnson Matthey, UK

[§]Eindhoven University

[∥]ION-TOF

 $^{^{\}perp} \text{ESRF}$

[#]MAX IV Laboratory

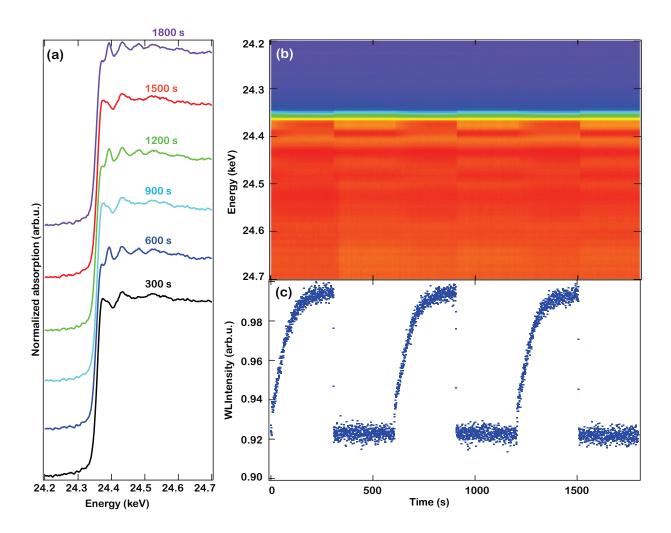


Figure S2: XAS spectra recorded during consecutive 300 s oxidising (1.5 % $\rm O_2$) and reducing (2 % $\rm H_2$) periods over Pd-Pt/Al₂O₃ F800 at 360 °C.(a) XAS spectra recorded at the end of the oxidising and reducing periods. (b) Colour coded intensities of XAS spectra (blue:low intensity, red:high intensity) and (c) the XAS white line intensity at 24 372 eV.

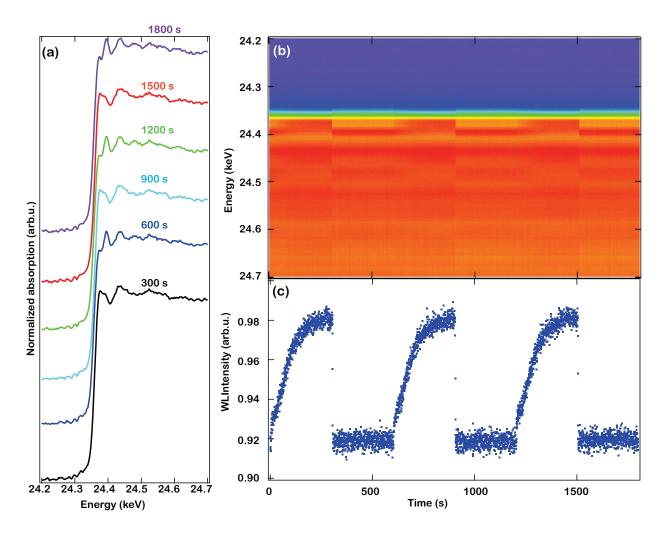


Figure S3: XAS spectra recorded during consecutive 300 s oxidising (1.5 % O_2) and reducing (2 % H_2) periods over Pd-Pt/Al₂O₃ L800 at 360 °C.(a) XAS spectra recorded at the end of the oxidising and reducing periods. (b) Colour coded intensities of XAS spectra (blue:low intensity, red:high intensity) and (c) the XAS white line intensity at 24 372 eV.