Support information

Magnetic manipulation of molecules on a non-magnetic catalytic surface

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Materials and Methods: The material used in this report was composed of Co cores (40-50 nm), covered with a thin carbon layer from TurboBeads to which we deposited Pt nanoparticles by means of wet impregnation. The average Pt diameter was 4-5 nm, verified by transmission electron microscopy (TEM). A representative sample is depicted in Fig. S1 and the average size was estimated from 50 nanoparticles.



Fig. S1. TEM imagine of Pt on carbon coated Co nanocore.

The RIXS experiments were performed at the SuperXAS beamline of the Swiss Light Source, Switzerland. The X-ray beam delivered by a superbend 2.9 Tesla bending magnet was monochromatized by means of a channel-cut Si (111) monochromator. The higher harmonics of the monochromator were rejected by means of a Rh-coated mirror operated at 3 mRad incident angle. Downstream the monochromator, the X-ray beam was focused down to ~100x100 μ m² by means of a Rh-coated torroidal mirror. For X-ray energies around the Pt L₃-edge the setup provides an energy resolution for incoming X-rays of about 1.5 eV and a flux of 5x10¹¹ photons/s. The X-ray fluorescence from the sample was

recorded with a von Hamos type spectrometer operating in Ge (660) crystal diffraction and at Bragg angle of 80 degree. A detailed description of the spectrometer setup can be found in Szlachetko et al. *Rev. Sci. Instrum.* **83**, 103105-103107 (2012). The sample was loaded into a thin 3 mm capillary reactor, and connected to a gas system. The catalyst was reduced in situ in hydrogen for 15 min at 300 °C. Prior to that the reactor was cooled in a flow of He to prevent reoxidation and kept under it for the duration of the experiments. RIXS maps changes due to the presence of a magnetic field and/or CO (1% in He) were measured at room temperature. The magnetic field was applied with the help of an electromagnet, which could be switched from 0 to 50 mT.



Fig. S2. (A) Physical process behind RIXS measurements; (B) Schematic representation of the experimental setup.

Calculations of RIXS maps

Theoretical calculations were performed according to what has been published elsewhere (O. V. Safonova, et al. *J. Phys. Chem.* B **110**, 16162-16164 (2006)) using a cluster of Pt₆. The DOS functions for Pt, Pt-CO atop and Pt-CO bridged geometries were computed by means of the FEFF9.0 code. The DOS functions were then used to calculate the RIXS planes by means of the generalized Kramers-Heisenberg formula developed by Tullki and Aberg (J. Tulkki and T. Aberg 1982 J. Phys. B: At. Mol. Phys. 15 L435). The energies and widths of the initial/final electronic states (i.e. $2p_{3/2}$ and $3d_{5/2}$) were taken from tabulated values (J. L. Campbell, At. Data Nucl. Data Tables 77, 50 (2001), R.D. Deslattes et al., Rev. Mod. Phys. 75, 35 (2003)). The calculated RIXS planes for Pt, Pt-CO atop and Pt-CO bridged adsorption are plotted in Figure.S4.

The experimental RIXS map differences were fitted by means of a least-square fitting method using the theoretical RIXS planes as references:

 $(A_0 \cdot Pt - A_1 \cdot Pt_{CO-atop})_{theoretical} \rightarrow (Pt - Pt_{CO})_{experimental}$

 $(B_0 \cdot Pt_{CO-atop} - B_1 \cdot Pt_{CO-bridged})_{theoretical} \rightarrow (Pt_{CO} - Pt_{CO with B=50mT})_{experimental}$

The A and B parameters stand for contribution of Pt, $Pt_{CO-atop}$, $Pt_{CO-bridged}$ signals to the intensity of the measured RIXS planes, and were kept free during the fitting procedure. The applied procedure allows for determination of the contribution of adsorption geometry to the measured RIXS signal and provides information about the relative concentrations of detected species. From the fitting, a contribution of 8.6% for A1 and 11% for B1 was obtained. As shown in the manuscript (Fig. 1 and 2), the calculated RIXS map differences estimated theoretically agree quantitatively with the experimental RIXS signal difference.



Fig. S3. Experimental RIXS maps. (*left*) Bare Pt; (*center*) CO adsorbed on Pt; and (*right*) CO adsorbed on Pt in the presence of a magnetic field (50 mT).



Fig. S4. Calculated RIXS maps. (*left*) Bare Pt_6 ; (*center*) CO adsorbed atop on Pt_6 ; and (*right*) CO adsorbed bridge site on Pt_6 .

The catalytic CO oxidation test was performed in a plug flow reactor using a gas mixture of 1% CO and 2% O_2 in Ar (total flow 30 mL/min). The catalyst was reduced in situ in hydrogen for 15 min at 300 °C, prior to reaction. The reaction outlet was analyzed by a quadrupole mass spectrometer (Hiden). The reaction temperature was kept at 120 °C because it was the temperature at which ~10% overall conversion was attained, on the basis of the light off experiments. The catalyst revealed the classic light-off curve shape with a light-off temperature of 175-190 °C corresponding to 50% conversion. The experiments in the presence of a magnetic field were run at 120°C to reactions to avoid mass transfer limitation, i.e., under differential conditions.