

# A detailed picture of CO oxidation on metal surfaces revealed by ambient pressure x-ray photoelectron spectroscopy

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In this contribution, we will demonstrate how a detailed and quite complete picture of the CO oxidation reaction can be obtained with ambient pressure x-ray photoelectron spectroscopy (APXPS) for three different metal surfaces: Pt(111), Ir(111), and Pd(100).

For the two first surfaces, chemisorbed phases form both when the surface is inactive and active [1]. In particular, we will focus on the phase transition from the inactive to the active state and give a detailed picture of the phases formed in this regime. Where Pt(111) either is inactive and CO covered or active and O covered, Ir(111) exhibits a transition state with co-existing chemisorbed O and CO (see fig. 1). The observed structural differences are explained in terms of DFT-calculated adsorption energies. For Pt(111) the repulsive CO-O interaction makes co-existing chemisorbed CO and O unfavourable, while for Ir(111) the stronger O and CO adsorption allows for overcoming the repulsive interaction.

In contrast, to Pt(111) and Ir(111) where chemisorbed phases are formed a thin surface oxide is formed on Pd(100) when the surface is active [2]. We will discuss how the formation of this surface oxide leads to hysteresis in the CO<sub>2</sub> formation during heating and cooling cycles well visible in a flow cell setup.

Finally, we will demonstrate how it is possible to measure the gas composition above the sample surface directly with APXPS and compare our results to recent planar laser-induced fluorescence (PLIF) measurements used to simulate APXPS experiments [3].

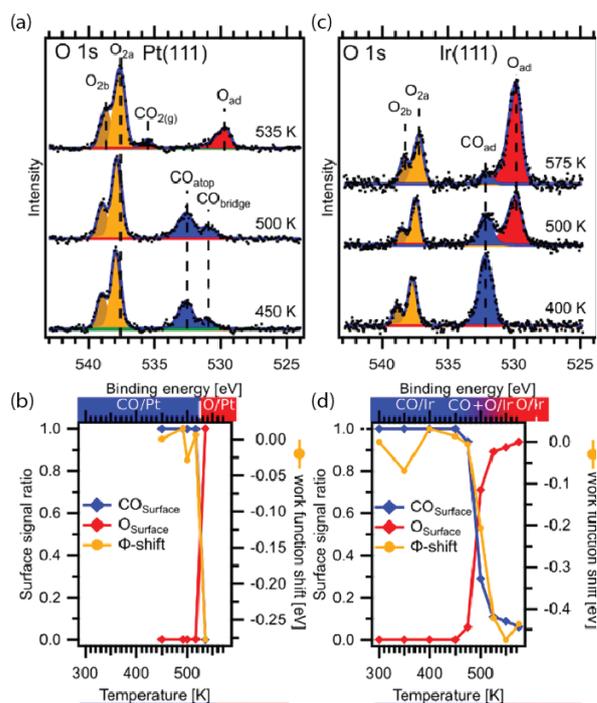


Figure 1: (a) O 1s APXPS spectra acquired in a 1:9 CO:O<sub>2</sub> mixture at 0.25 mbar over Pt(111) at different temperatures, (b) the ratio between the surface species and workfunction shift (c-d) Corresponding figures for Ir(111)

## References:

- [1] N Johansson, et al., Jour. Phys. Cond. Matt, **29**, 44 (2017)
- [2] V. R. Fernandes et al., ACS cat, **6**, 4154, (2016)
- [3] J. Zhou et al., Catalysts, **7**, 29 (2017)