ESRF	**Experiment title:** "Unbinding" a large aromatic adsorbate from a metal surface by metal co-adsorption	**Experiment number**: SI-1829
Beamline:	**Date of experiment**: from: 18/02/2009 to: 24/02/2009	**Date of report**: 15/02/2010
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Report: The aim of the experiment SI-1829 was to study the unbinding process of PTCDA molecule at Ag(110) surface upon co-adsorption of K atoms by means of NIXSW technique. It was expected that alkali atoms interacting with oxygen atoms of molecules will partially release them from the interface bonding with the substrate. This should be seen in an overall increase of the PTCDA adsorption height and a decrease of the molecular distortion. As a reference, we used the pure molecular phase of (3×3)PTCDA/Ag(110) to compare the molecular bonding distances and distortions before and after reaction with potassium.

NIXSW experiments were performed on ordered monolayers of PTCDA/Ag(110) and the mixed phase of PTCDA+K/Ag(110) according to preliminary developed preparation protocol (Fig. 1). In the experiments, 5 sets of NIXSW data were collected for C1s core level and 6 for N1s core level for PTCDA/Ag(110) and 9 sets for C1s

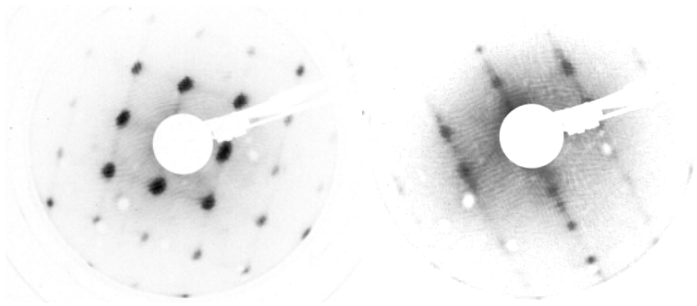

Figure 1. LEED images of (3×3)PTCDA/Ag(110) and PTCDA+K/Ag(110)

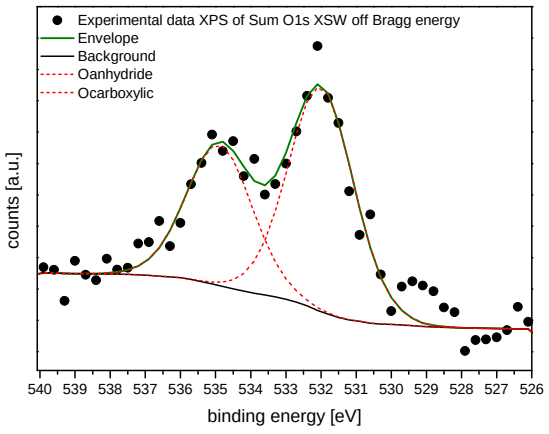

Figure 2. Experimental XPS spectrum (dots) and corresponding fit (lines) of O1s core level

and K2p line, 10 for K1s, and 10 for O1s for K+PTCDA/Ag(110). NIXSW for silver related core levels and Auger lines was recorded as well to control the quality of substrate crystallity.

The resolution of the acquired photoemission spectra for O1s line was sufficient for performing the differential analysis, i.e. separating the contributions of carboxylic and anhydride oxygens. To develop the corresponding fitting model (Fig.2), high resolution photoemission spectra of O1s peak were recorded.

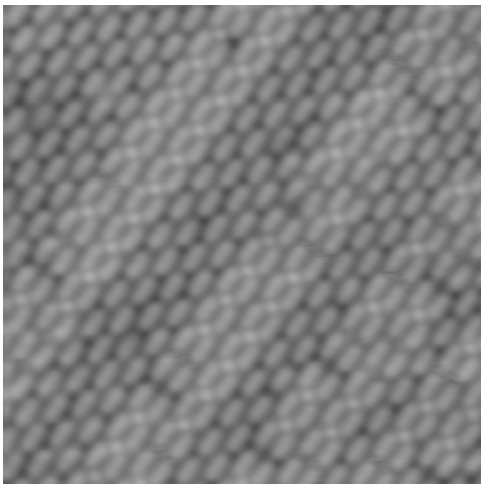

Figure 3. PTCDA+K/Ag(110). Initial stage of the phase transformation at very low K coverage

Analysis of NIXSW data for the pure molecular phase of PTCDA on Ag(110) demonstrated a perfect reproducibility of the results obtained in different experiments. The adsorption height and geometry of PTCDA molecule measured in the experiment SI-1829 was found very close to what was measured during the previous experiment SI-1645 devoted to adsorption of PTCDA on silver surfaces of different orientations – (111), (100) and (110). The difference is within the experimental accuracy (<0.05 Å). As it was expected, the thermal activated (annealing at 180°C) reaction of PTCDA molecules with adsorbed potassium atoms results in a noticeable change of the bonding distance and relaxation of internal molecular geometry [1].

To solve the adsorption model completely, i.e. to define the exact position of potassium atoms in the layer after reaction, additional studies with complementary in-house methods are currently in progress. Structural investigations are performed by high resolution SPA-LEED (Bonn) and low temperature scanning tunneling spectroscopy (Jülich) (Fig. 3), while electronic properties are studied with angle resolved UPS (Jülich). The joint publication on results of these experiments will be prepared [1].

[1] G. Mercurio, O. Bauer, A. Dehley, R. Temirov, S. Soubatch, M. Sokolowski, F.S. Tautz, *to be submitted*