

**Experiment title:**Interplay between vertical adsorption structure of organic molecules and the surface work-function: PTCDA/Cu₃Au(111)**Experiment number:**

SI-2186

Beamline:	Date of experiment: from: 22/02/2011 to: 01/03/2011	Date of report: 05/04/2011
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Report: In the SI-2186 experiment, we planned to investigate the adsorption geometry of PTCDA on Cu₃Au(111) with normal incidence X-ray standing wave technique (NIXSW). The main aim of the study was to verify a formulated empirical rule about interplay between adsorption height of organic molecules and the surface work-function (cf. [1], progress report on SI-1645).

During experiment, we prepared a monolayer of PTCDA on Cu₃Au(111) surface according to preliminary developed preparation protocol (Fig.1). Carrying out X-ray photoemission spectroscopy, needed for developing of fitting model for C1s and O1s core levels for proper evaluation of NIXSW data, we observed a minor but noticeable shifts of corresponding peaks during first 15 minutes of X-ray exposure. We interpreted this as a beam damage of organic layer induced by

electrons emitted by substrate elements under 2.865 keV (Bragg energy of Cu₃Au(111)) X-ray excitation. Since the currently used at ID32 beam line acquisition software (SPECSlab 2) controlling the new SPECS Phoibos 225 analyser does not allow an

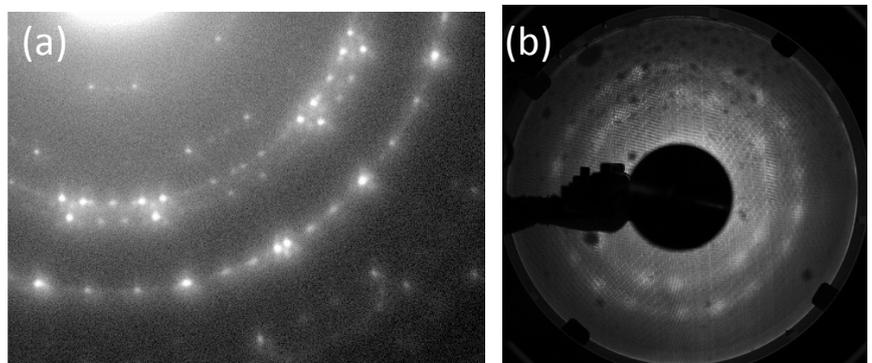


Fig. 1 (a) SPA-LEED (University of Bonn) and (b) conventional LEED (ID32, ESRF) of 1ML PTCDA on Cu₃Au(111)

arbitrary choice of used acquisition time due to significant dwell times, we developed a way to proceed with NIXSW such that at each “fresh” spot of PTCDA/Cu₃Au(111) sample only two XPS spectra (5 minutes each) at different photon energies from one NIXSW sequence were recorded; after that the sample was automatically moved to another “fresh” spot until the whole required range of photon energies ($E_{\text{Bragg}} \pm 3\text{eV}$) was used. Thus an intact state of PTCDA/Cu₃Au(111) interface was investigated with NIXSW. For comparison, NIXSW dataset at already irradiated sample spot was acquired as well. These experimental data are under evaluation now.

Using the high stability and high transmission of recently installed at ID32 electron analyser SPECS Phoibos 225, during SI-2186 experiment we also investigated the adsorption height of PTCDA molecule at Ag(100) surface. Previous attempts to study the PTCDA/Ag(100) interface (SI-1451, SI-1645) failed because of low stability of the previously used analyser. During SI-2186 experiment we successfully prepared a monolayer of PTCDA on Ag(100) and obtained a full set of XPS and NIXSW data on it. Corresponding data are under evaluation.

[1] A. Hauschild *et al.*, PRB 2010. **81**, 125432.