ESRF	**Experiment title:** Structural investigations of the adsorption of large organic molecules on metal surfaces	**Experiment number**: SC-1372
Beamline:	**Date of experiment**: from: 04.06. to: 14.16.2005 and 25.01. to: 01.02.2005 and 16.06. to: 22.06.2004 and 18.11. to: 27.11.2003	**Date of report**:
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Report:

The main results from this long term project are published in the following papers:

C. Stadler, S. Hansen, F. Pollinger, C. Kumpf, E. Umbach, T.-L. Lee, J. Zegenhagen, „Structural investigation of the adsorption of SnPc on Ag(111) using normal-incidence x-ray standing waves“, Phys. Rev. B **74**, 035404 (2006)

Abstract: The bonding of tin(II)-phthalocyanine (SnPc) on Ag(111) was studied using the normal incidence x-ray standing wave technique. For an incommensurate monolayer structure at room temperature, it was found that the SnPc molecules adsorb in a “Sn-down” geometry, i.e., the Sn atoms lie below the molecular plane. A significant bending of the benzene rings toward the surface indicates that these rings contribute to a chemisorptive bonding of the molecule to the surface. This effect is found to be even enhanced for another phase, a commensurate submonolayer structure that is only stable at low temperature. In this phase, the molecules are located significantly closer to the surface in a mixed “Sn-up”-“Sn-down” configuration. Nondipolar contributions to the photoelectron yield were also investigated and taken into account.

J. Stanzel, W. Weigand, L. Kilian, H.L. Meyerheim, C. Kumpf, E. Umbach, “Chemisorption of NTCDA on Ag(111): a NIXSW study including non-dipolar and electron-stimulated effects”, Surf. Sci. **571**, L311 (2004)

Abstract: The adsorption of one monolayer of 1,4,5,8-naphthalene-tetracarboxylicacid-dianhydride (NTCDA) on the Ag(111)-surface was studied using the normalincidence X-ray standing waves (XSW) technique. Results regarding two key-issues are presented: Most prominent, the precise adsorbate–substrate bonding distance could be evaluated to 3.02 ± 0.02A ˚ (for the ‘‘relaxed monolayer’’-structure). This value is significantly smaller than a van der Waals bonding distance and clearly indicates the chemisorptive bonding character. Concordant results were obtained from both O 1s photo- and O KLL Auger electron emission. This was enabled by the development of a data analysis procedure—the second issue addressed—which takes into account non-dipolar contributions to the photoemission as well as electronstimulated Auger excitations. The latter effect adds a fraction to the total Auger yield being as high as 50% and hence may be important for any XSW study using Auger signals.

Furthermore, this long-term project (together with subsequent projects) has set the basis for other publications in high-indexed journals:

C. Stadler, S. Hansen, I. Kröger, C. Kumpf, E. Umbach, „Tuning intermolecular interaction in longrange-ordered submonolayer organic films“, Nature Physics **5**, 153 (2009)

C. Stadler, S. Hansen, A. Schöll, T.-L. Lee, J. Zegenhagen, C. Kumpf, E. Umbach, „Molecular distortion of NTCDA upon adsorption on Ag(111): a normal incidence x-ray standing wave study “, New J. Phys. **9**, 50 (2007)