ESRF	**Experiment title:** Structural investigations of the adsorption of large organic molecules on metal surfaces	**Experiment number**: SI-1377
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Report:

The results obtained in this project have contributed to the following publications:

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)

Abstract: We investigated the adsorption geometry of the model system NTCDA (1,4,5,8-naphthalin-tetracarboxylicacid-dianhydride) on Ag(111) using the normal incidence x-ray standing wave (NIXSW) technique. For the relaxed monolayer structure a significant vertical distortion of the molecule is found upon adsorption. The carboxylic oxygen atoms at the corners of the molecule are located 0.25(3)Å closer to the topmost Ag atoms than the naphthalene core at 2.997(16)Å. This distortion effect is similar to that of the larger molecule (3,4,9,10-perylene tetracarboxylicacid-dianhydride) (PTCDA)/Ag(111) (Hauschild A et al 2005 Phys. Rev. Lett. 95 209602), but the chemisorptive bonding is weaker. Our structural investigation is based on photoelectron and Auger emission NIXSW data, the independent measurement of which allows us to correct in a self-consistent way for non-dipolar contributions to the photoelectron yield as well as for electron induced Auger processes, two effects which may significantly influence the structural results if not considered.

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.