



	Experiment title: Structural investigations of the adsorption of large organic molecules on metal surfaces	Experiment number: SI-1529
Beamline:	Date of experiment: from: 07.03. to: 12.03.2007	Date of report:
Shifts:	Local contact(s): Tien-Lin Lee	<i>Received at ESRF:</i>
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Report:

The most prominent result from this and the subsequent project SI1647 has been published recently in Nature Physics:

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

The future success of organic electronic devices strongly depends on the ability to tailor the properties of thin films and interfaces. This calls for well-ordered thin films. However, their properties are dominantly influenced by the formation of the first molecular layer representing a template for further growth. The development of the first layer—in turn—depends on the fine balance of molecule–substrate and molecule–molecule interaction. The latter is usually attractive owing to van derWaals forces and causes the formation of islands and small crystalline grains. Here, we report on organic adsorbates exhibiting a repulsive intermolecular interaction. With increasing coverage, Sn-phthalocyanine molecules continuously rearrange on Ag(111) in a series of ordered superstructures. They always fill the surface terraces homogeneously and maximize the domain size. Thicker films also exhibit extremely large, monocrystalline grains and potentially enable bulk-like properties for thin films. The intermolecular interaction can be tuned by cooling and becomes attractive below 120 K.

Another part of the results from this beamtime are published in

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 $0.25(3)\text{\AA}$ closer to the topmost Ag atoms than the naphthalene core at $2.997(16)\text{\AA}$. 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.