


**Experiment title:**

X-ray Standing Wave Investigation of Azobenzene-triazatriangulenium Derivatives on Au(111)

**Experiment number:**

SI-2007

**Beamline:**

ID32

**Date of experiment:**

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**Date of report:**
**Shifts:**

5

**Local contact(s):**

Blanka Detlefs

*Received at ESRF:*

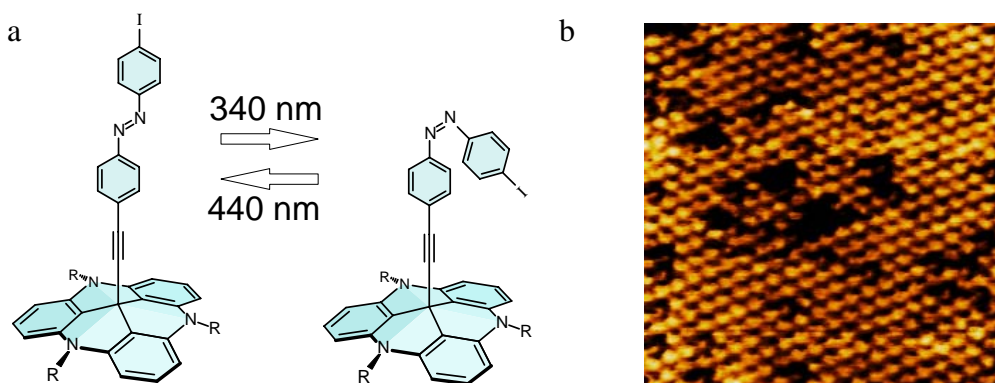
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**Report:**

Photowitchable molecules may reversibly change their conformation and thus their properties through external stimulation by light. They are of great interest to nanoscale functional devices, e.g. in information storage, sensors, drug delivery, and molecular machines [1]. In many of these applications the functionality is achieved through binding these molecules on a substrate. Azobenzene is one of the best known among these switchable molecules and has been extensively studied [1,2]. It undergoes a reversible conformational change from *trans* to *cis* upon illumination with UV light and a backisomerisation to the *trans* state upon illumination with blue light.

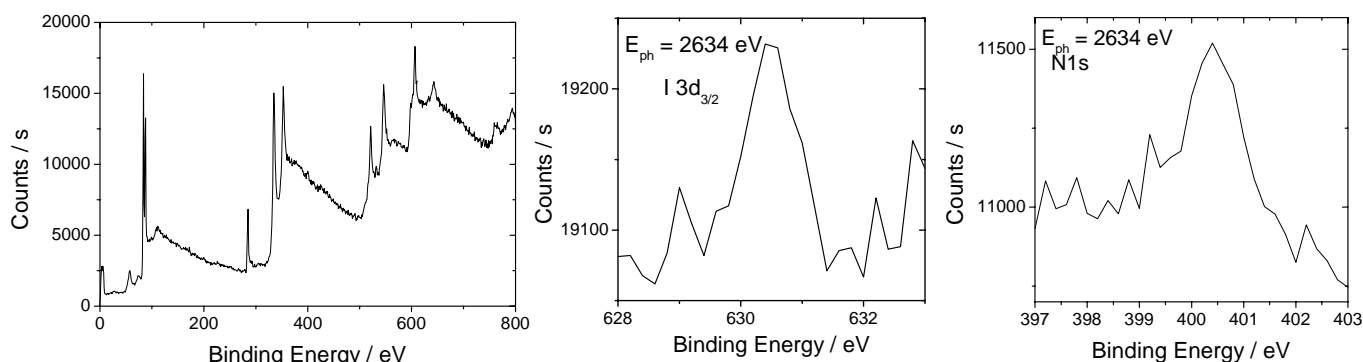


**Figure 1:** (a) Iodine-functionalized Azo-TATA (I-Azo-TATA) molecule in *trans* and *cis* conformation. (b) STM image of Azo-TATA on Au(111) (25 x 25 nm).

**Experiment:**

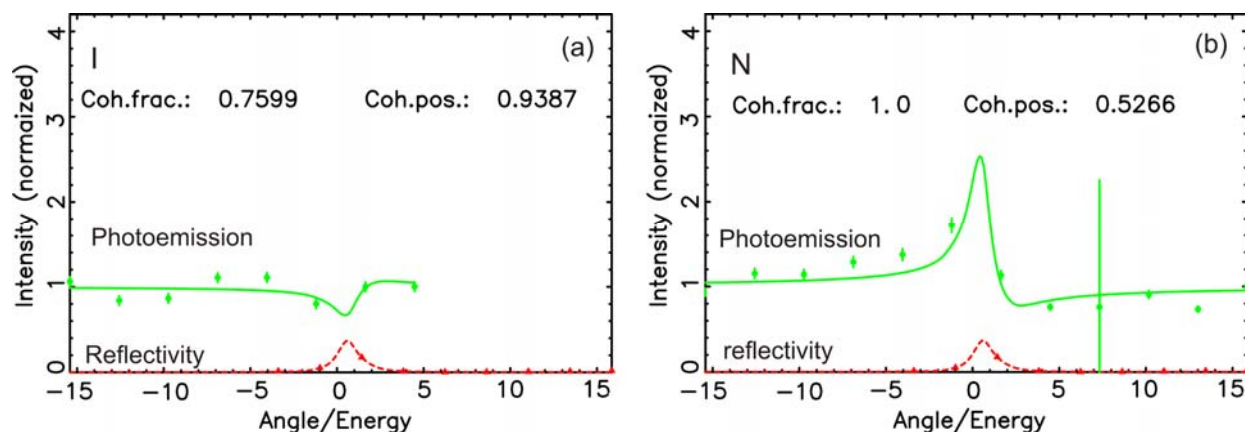
X-ray standing wave investigations were carried out on ID32. The high quality Au(111) single crystal substrate was prepared by flame annealing and then immersed into a I-Azo-TATA containing solution to allow formation of the self assembled monolayer [4]. The samples were then transferred into the vacuum chamber via a fast entry load lock. Because of the mosaic spread of Au crystals, the measurement was carried

out in backscattering geometry and thus Auger and photoelectrons were monitored to obtain the SXW profiles, therefore, vacuum conditions were required. The monolayer quality and composition were monitored by X-ray photoelectron spectroscopy. Measurements at the Au(111) reflection show a high coherent fraction confirming the monolayer quality and feasibility of the measurements. Due to the low I intensity available it was only possible to record one XSW in the short time available. The XPS measurements showed that all expected components were present; see the overview spectrum in fig. 22. The core level measurements clearly revealed a signal from the iodine head group (fig. 3b) and the nitrogen (fig. 3c) proving experimental feasibility.



**Figure 3:** XPS data collected ( $E_{ph} = 2634$  eV) (a) overview spectrum, (b)  $I_{3d}$  core level and (c)  $N_{1s}$  core level.

The standing X-ray field was generated as the energy was varied about the Bragg energy Au(111) reflections at a photon energy of 2.6 keV, reflected beam intensities were recorded along with intensities of the I(3d) and later N(1s) photoelectrons with the hemispherical electron analyser. XSW curves for the I(3d) and N(1s) core levels from an Iodine-functionalized Azo-TATA monolayer on Au(111) were collected as seen in fig. 3a and b. Fits to the data give preliminary values for the coherent fraction of 0.76 and 1.0 and coherent position of 0.93 and 0.52 for I and N respectively. More data points are required to confirm these values but they indicate that XSW's are a useful tool for observing this system.



**Figure 2:** (a) Rocking curve and fluorescence curve of I collected at ID32. coherent fraction 0.76, coherent position 0.94. (b) Rocking curve and fluorescence curve of N collected at ID32 coherent fraction 1, coherent position 0.52.

## References

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2. K. Ichimura, S.K. Oh, M. Nakagawa, Science, **288** (2000) 1624.
3. U. Jung, et al., J. Electroanal. Chem, **619** (2008) 152.
4. B. Baisch, et al., J. Am. Chem. Soc, **131** (2009) 442.
5. S. Kuhn et al. PCCP, DOI:10.1039/B922882A (2010).