

**Experiment title:**

Thermal switching of molecular dipoles measured by X-ray standing waves

Experiment number:

SI-2073

Beamline:

ID 32

Date of experiment:

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Shifts:

18

Local contact(s):

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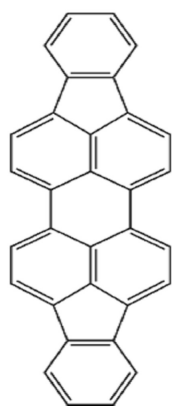
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*Chiba University, Graduate School of Advanced Integration Science, Japan***Report:****1. Introduction**

During this beamtime we proposed to study the thermal switching of molecular dipoles by X-ray standing waves (XSW) for the case of Gallium-Chlorine Phthalocyanine (GaClPc). This study requires a very precise controlling of the temperature. Due to the newly installed preparation chamber at ID32 it was not possible yet to adjust the temperature with the needed precision. We therefore decided to determine the bonding distance of diindenoperylene (DIP) adsorbed on three noble metal surfaces (Cu(111), Ag(111) and Au(111)).



In the following a short summary is given of the results which were obtained during beamtime SI-2073.

2. XSW measurements of DIP on Cu(111), Ag(111) and Au(111)

For each Cu(111), Ag(111) and Au(111) substrate two films of DIP with a coverage around one monolayer were prepared by thermal evaporation. XPS spectra of the C1s peak were taken before and after the XSW measurement in order to check possible beam damage. As can be seen exemplarily from Fig. 2b for DIP/Ag(111) by comparing the XPS scans of C1s before (blue) and after

Figure 1: Chemical structure of diindenoperylene(DIP).

(red) the XSW scan, no change of the shape is visible. Thus we conclude that there was no relevant molecular damage induced by the X-ray-beam.

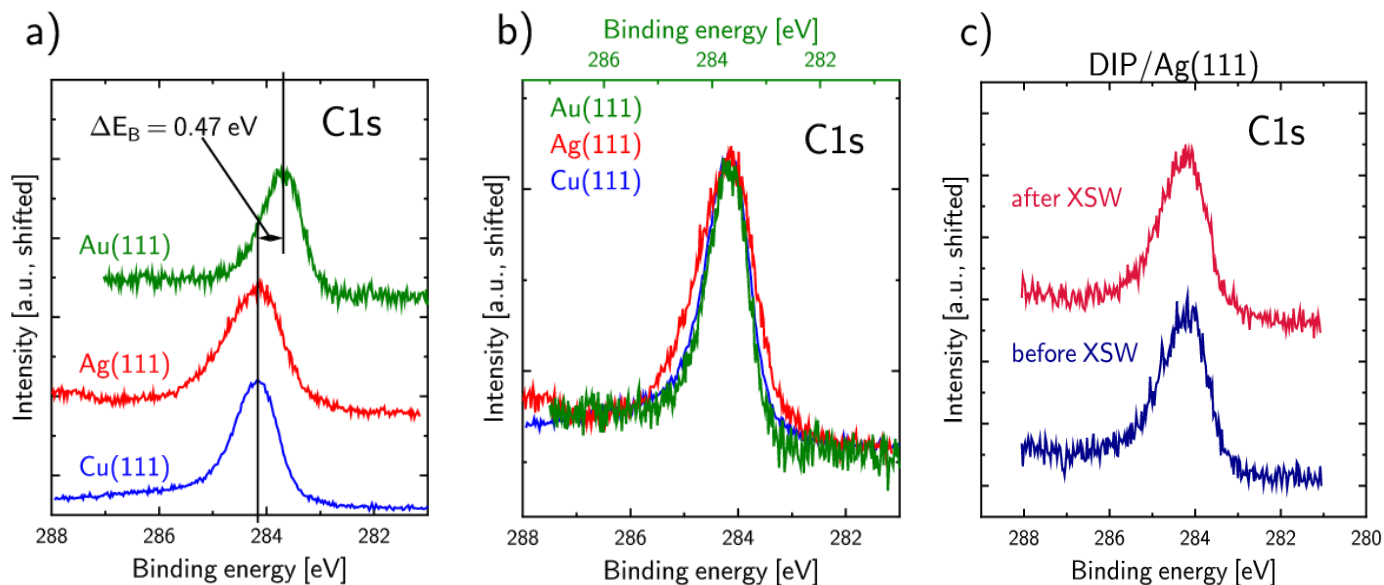


Figure 2: XPS spectra of C1s measured on a (sub-)monolayer of DIP on Cu(111), Ag(111) and Au(111). a) The C1s peak of DIP/Au(111) (green curve) is shifted towards lower binding energies compared to DIP on Cu(111) and on Ag(111) (blue and red curve, resp.). b) Shape of the C1s peak measured on the three metal surfaces. The green curve is shifted towards higher binding energies. c) C1s for DIP/Ag(111) before (top, red curve) and after (bottom, blue curve) a XSW measurement.

Looking at high resolution XPS of the C1s peak for the three systems, a different binding energy of DIP on Au(111) was detected compared to DIP on Cu(111) and Ag(111). This difference in binding energy is 0.47 eV (Fig. 2a). Also the shape of the C1s peak was not the same for the three systems (Fig. 2b). On Ag(111) (red curve) we observe a broader peak, which may be induced by molecules adsorbed as a second layer or by possible tilted molecules.

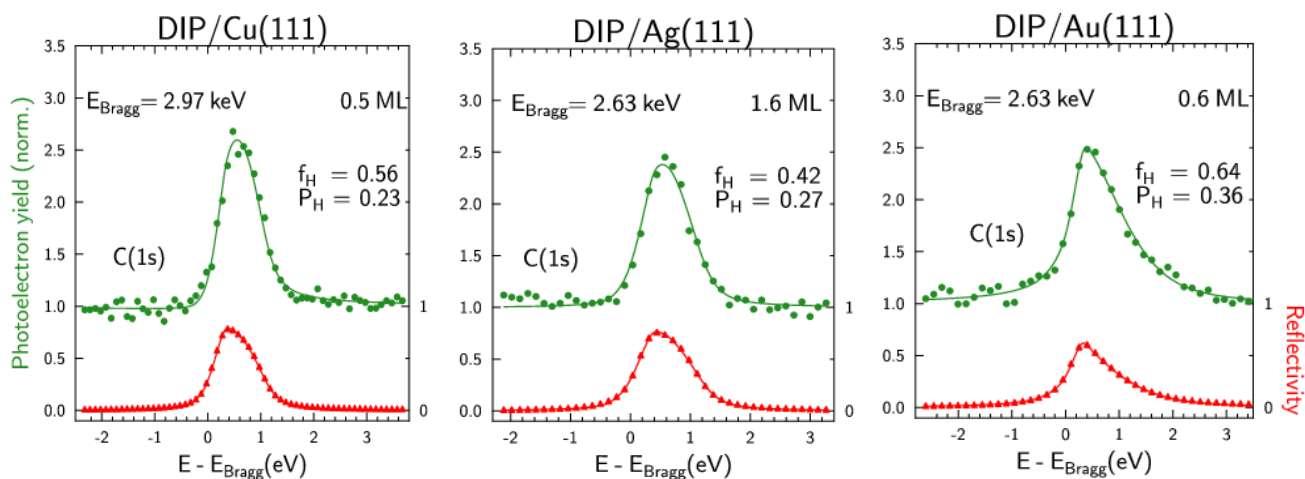


Figure 2: C1s XSW data of DIP on Cu(111), Ag(111) and Au(111) (from left to right). Green and red points are data of photoelectron yield and reflectivity respectively. Both are fitted by theoretically, indicated by the solid line.

XSW measurements of carbon were performed at several spots for each prepared film for tests of reproducibility. Every conducted XSW scan is listed in the Argand diagram (Fig. 3).

We observe a substrate-dependent bonding distance of DIP. The average bonding distance of the DIP molecule on Cu(111) is around 2.5 Å. On Ag(111), DIP adsorbs at a bonding distance of around 3.0 Å. The largest bonding distance is observed for DIP on Au(111) (around 3.2 Å). Not only the bonding distances but also the coherent fractions seem to depend on the substrate although the error bar is not negligible. The coherent fraction is influenced by thermal vibrations, the degree of distortion of the molecule as well as vertical disorder, and therefore it is difficult to address the different values coherent fractions of the three systems to one specific origin.

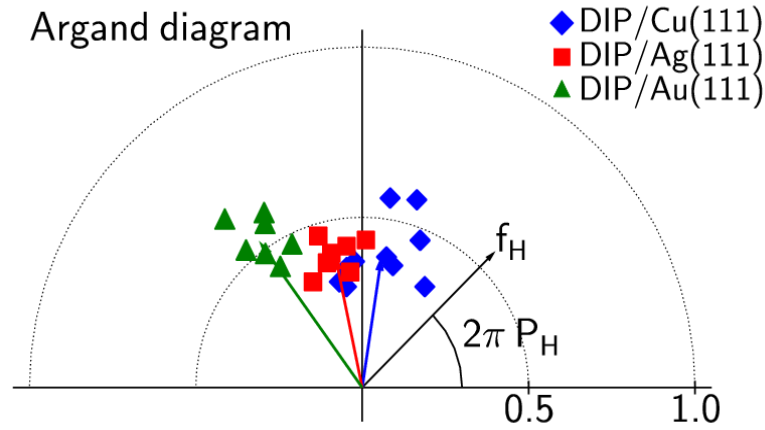


Figure 3: Argand diagram containing all conducted XSW measurements of DIP on Cu(111), Ag(111) and Au(111) (blue, red and green markers resp.). One marker represents a XSW scan. The distance to the origin is given by the coherent fraction f_H while the angle to the x-axis is proportional to the coherent position P_H . The coloured arrows illustrate the averaged coherent position and coherent fraction.

We wish to thank our local contacts for the excellent support at ID32.