

**Experiment title:**

Molecular Adsorption and Interface Dipoles of Pentacene Studied by XSW

Experiment number:

SI-1526

Beamline:

ID 32

Date of experiment:

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03/09/2007

Shifts:

18

Local contact(s):

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As outlined in the proposal, the purpose of the experiments at ID32 was to measure bonding distances and conformation of pentacene (PEN; Fig. 1) and perfluoro-pentacene (PFP; Fig. 1) on noble metal surfaces. In combination with other complementary techniques the X-ray standing wave (XSW) measurements will establish a fundamental understanding of the two prototypical organic semiconductors in the monolayer regime [1].

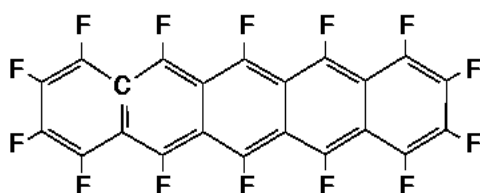
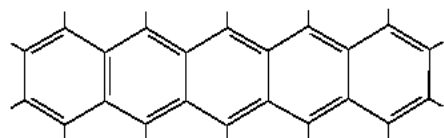


Illustration 1: Chemical structure of PEN and PFP

We intended to use Au(111) and Cu(111) single crystals, but unfortunately the quality of our Au(111) crystal did not permit meaningful XSW measurements. The Cu(111) substrate, however, turned out to be of high quality, with the a normal incidence rocking width of ~ 0.90 eV (close to the intrinsic value), and could successfully be used for XSW measurements.

Below we give a short summary of results from the beam-time (SI-1526) at ID32.

2. XPS and XSW measurements on monolayers of PEN and PFP

Several films of PEN and PFP with different coverages in the sub-monolayer and monolayer regime were prepared at a substrate temperature of $T=80$ °C. We used both C(1s) carbon signals shown in Fig. 2 and the F(1s) fluorine signal for our XSW experiments.

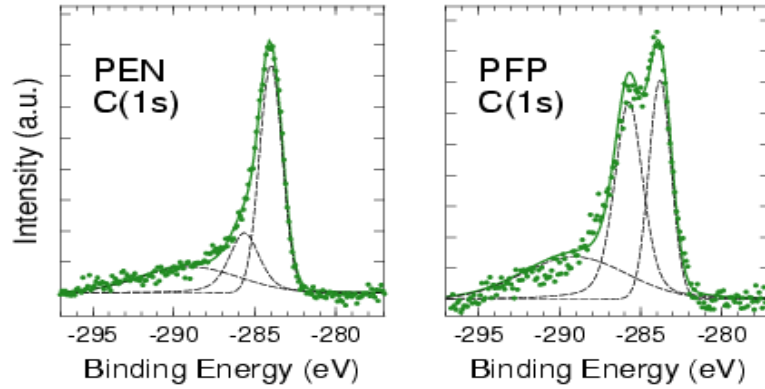


Illustration 2: Carbon XPS signals from a sub-monolayer of PEN and PFP on Cu(111). Note the splitting of the C(1s) for PFP which corresponds to the different chemical environments of the carbon atoms (C-C versus C-F bonded).

Due to the improved stability of the new monochromator we were able to acquire high quality XSW data. The characteristic variation of the photo electron yield in the X-ray interference field provides the coherent positions P_{eff} and coherent fractions f_{eff} for the atoms in the PEN and PFP molecules on Cu(111), see Fig. 3 and Tab. 1. In the data analysis we followed the procedures established in [2]. After converting these data into distances and applying non-dipole corrections we find an (average) C-Cu bonding length of (2.34 ± 0.02) Å for PEN and (2.98 ± 0.07) Å for PFP, *i.e.*, a difference of 0.64 Å between the carbon cores of these two adsorbate systems on Cu(111). As we find that the fluorine atoms of PFP reside at a distance of (3.08 ± 0.04) Å, the XSW results suggest that the PFP molecule does not adsorb in a planar configuration on Cu(111).

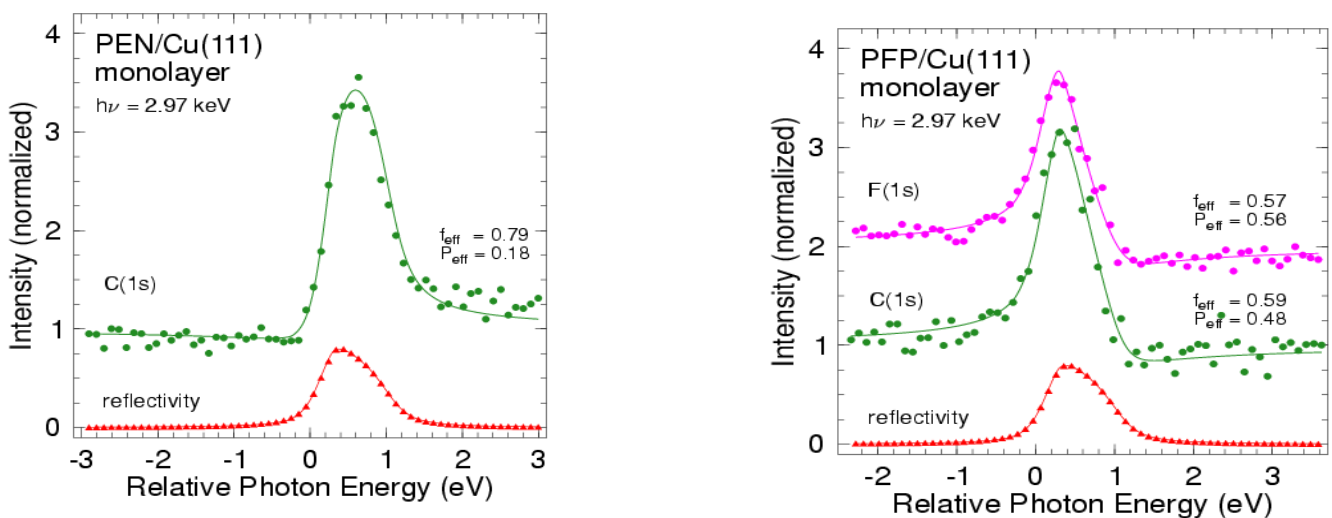


Illustration 3: X-ray standing wave scans obtained on sub-monolayers of PEN and PFP on Cu(111). The symbols represent the photo electron yield (circles) and reflectivity (triangles) data measured on both adsorbate systems. The solid lines show least-square fits based on dynamical diffraction theory which provide the coherent position P_{eff} and coherent fraction f_{eff} for each element. The characteristic shapes of these curves reveal the different adsorption distances d of PEN and PFP, whereas the deviation of the coherent fractions from unity is related to disorder in the adsorbate system.

3. Summary

We were able to measure all relevant data for PEN and PFP on Cu(111), see Tab. 1. The surprisingly big difference between the bonding distance of PEN and PFP have been found. These results in good agreement with complementary measurements using photoemission and scanning tunneling microscopy data.

	PEN/C(1s)	PFP/C(1s)	PFP/F(1s)
f_{eff}	0.79	0.59	0.57
P_{eff}	0.18	0.48	0.58
f_{H}	0.55	0.41	0.41
P_{H}	0.12	0.42	0.47
d_{H}	$(2.34 \pm 0.02) \text{ \AA}$	$(2.98 \pm 0.07) \text{ \AA}$	$(3.08 \pm 0.04) \text{ \AA}$

Table 1: XSW results for PEN and PFP on Cu(111) including the non-dipole correction [2].

A manuscript with all results has been submitted [3]. - We wish to thank our local contact for the excellent support on ID32.

4. References

- [1] N. Koch et al., "The effect of fluorination on pentacene/Au interface energetics and charge reorganization energy", *Adv. Mater.* **19** (2007) 112
- [2] A. Gerlach et al., *Adsorption-induced distortion of F₁₆CuPc on Cu(111) and Ag(111): An X-ray standing wave study*, *Phys. Rev. B* **71** (2005) 205425
- [3] N. Koch et al., "Strong distortion upon adsorption: Correlating molecular conformation and interface electronic structure", submitted