

## XSW feasibility study of C<sub>60</sub>Ph<sub>5</sub>–OH on Ag(1 1 1): combining hard X-rays, low Z and, low coverage

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### Abstract

We have undertaken a "proof of principle" Normal Incidence X-ray standing wave (NIXSW) experiment on a monolayer of C<sub>60</sub>Ph<sub>5</sub>–OH, a functionalised fullerene, on Ag(111) and show that it is indeed possible to use XSW in case of extremely low coverage of low Z elements such as oxygen. We find a tentative coherent fraction  $f_{co}$  of 30% and a coherent position  $D_{co}$  of 2.35Å.

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### 1. Introduction

The last few years have seen an explosion of activity in the field of molecular devices and nanotechnology, dealing with ever smaller structures and firmly incorporating organic molecules in areas of research traditionally associated with

inorganic solid state physics. Increasingly, the possibilities of self-assembled structures or atom-by-atom positioning are becoming feasible exploits for investigation and indeed applications [1,2]. It is then a natural consequence that this is accompanied by an increased demand for accurate determination of surface geometries and bonding of such assemblies. Certain real space techniques such as scanning tunneling microscopy (STM) are providing one important solution to this quest, however, there are situations where STM alone cannot provide the answer. For

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example, investigating the possibility of ordering of the caged atom within an endohedral fullerene with respect to the surface registry will require an alternative approach to the problem. In this case a solution can be provided by using the X-ray standing wave (XSW) technique as in, for example, Ref. [3]. Also, combining XSW with other techniques like near edge X-ray absorption spectroscopy (NEXAFS) and photoelectron spectroscopy (PES) is an excellent way of obtaining both electronic structure and geometry information. In short, one can say that even when several techniques are available to probe a certain query, much is to be gained from employing complementary techniques to that problem, as the shortcomings of one can be covered by another and thus much more accurate knowledge can be obtained.

The advantages of a technique like XSW, or normal incidence XSW (NIXSW) in our case, are clear: it can offer accurate determination of both height and lateral position of (sub)-monolayers of atoms on top of a substrate, measure buried interface layers, identify the position of impurities, and surface reconstructions. Furthermore, it can distinguish between signals from atoms of the same element in different chemical surroundings, as was demonstrated by exploiting the different species of phosphorous in co-evaporated PF, PF2 and PF3 which were found to occupy different absorption sites on Ni(111), as reflected in the 3 components that make up the P 1s peak in Ref. [4]. This also demonstrates that it is a technique that works well in the absence of long range order. For a complete analysis of the (NI)XSW technique there are many excellent reviews available, such as that by Woodruff et al. [5] and that of Zegenhagen [6]. Here, we will just give a concise description.

Starting with a suitable single crystal substrate with a well-known plane separation  $d$ , NIXSW essentially combines the use of the Bragg condition for X-rays with the X-ray absorption experienced by atoms embedded within the standing wave field set up by these photons. When the photon energy is scanned through the Bragg energy region, the X-ray absorption cross-section and, therefore, also the emission yield of photoelectrons or Auger electrons, will be modulated in a particular way,

depending on the position of the atom relative to the scattering planes. This yield  $Y_p$  can be described by

$$Y_p = 1 + R + 2\sqrt{R}f_{co} \cos(\phi - 2\pi D), \quad (1)$$

where

$$R = \left| \frac{E_H}{E_0} \right|^2 \quad (2)$$

is the reflectivity and  $E_0$  and  $E_H$  are the incident and Bragg-reflected electric fields of the photons which produce the standing wave of phase  $\phi$ . The information contained in this formula is  $D$ , the coherent position (in terms of the lattice spacing  $d$  of the crystal used as a substrate) and  $f_{co}$ , the coherent fraction i.e. the degree of order associated with a particular site occupation. Another effect, first described by Berman and Bedzyk, has to be included in this yield description [7], its origin lies in the polarization of the incident radiation which is not included in the above equation. A general formalism for the inclusion of both polarization and multipole effects was developed by Vartanyants and Zegenhagen [8]. Essentially it describes the asymmetry in photoelectron signal relative to the photon propagation direction, i.e. the difference in electron yields generated by the incoming and outgoing photon fields due to non-dipolar effects. This is an important consideration when using photoemission, instead of Auger, as the outgoing photoelectrons themselves have an angular intensity distribution and electron collection will always occur over a small, angular portion of the spherical half-dome above the sample. In the case of an initial s-state and normal incidence geometry for  $\sigma$ -polarized light Eq.(1) must be modified according to Ref. [8], which when cast in terms of an asymmetry parameter  $Q$ ,

$$Y_p = 1 + R \frac{(1+Q)}{(1-Q)} + 2f_{co}\sqrt{R} \frac{(1+Q^2 \tan^2 \Delta)^{1/2}}{(1-Q)} \times \cos(\phi + \psi - 2\pi D). \quad (3)$$

Where

$$\psi = \tan^{-1}(Q \tan \Delta) \quad (4)$$

and

$$\Delta = \delta_d - \delta_p, \quad (5)$$

$\delta_d$  and  $\delta_p$  are the partial phase shifts of the final electron p- and d-state.

This asymmetry factor can be substantial [9,10] and is particularly important when describing photoelectron emission from low  $Z$  elements, which have shallow core levels, relative to the high photon energies routinely used in NIXSW (2–4 keV), and therefore have an increased sensitivity to higher order effects. For example, in the case of monitoring the oxygen 1s signal of a bulk film of PTCDA ( $C_{24}H_8O_6$ ) on Ag(111) a value of  $Q = 0.31 \pm 0.03$  was found [11], which is consistent with expectations from calculations ( $0.306 < Q < 0.33$ ) [12]. This also brings us to a natural disadvantage of the NIXSW technique: the higher the photon energy the lower the cross-section for PES, and this effect is even more disadvantageous for low  $Z$  elements and shallow core levels. Therefore, with the current emphasis on organic molecules consisting mainly of C, N, O and H this could represent a serious constraint on the use of this technique. Another blow would be the demand for measurements on very low, sub-monolayer coverages of molecules. It has, however, already been established that the low  $Z$  elements themselves do not present a problem as long as there is sufficient coverage on the substrate, i.e. when the relative coverage of the element is close to a monolayer, signals still prove to be sufficient and conveniently measurable, like in the case of PTCDA [13]. Similarly, when the organic molecule incorporates a heavier element that can be used as a marker for the position and orientation of the molecule, like a rare earth ion in endohedral fullerenes, or a transition metal (TM) ion in TM-phthalocyanines, a relatively low coverage of that heavier element of the order of 0.03 ML is still sufficient for good NIXSW results [14]. Therefore, the real challenge for the standing wave technique on single crystal substrates currently lies with very low coverages of low  $Z$  elements. With this in mind, we have conducted a “proof of principle” study of  $C_{60}Ph_5-OH$ , a molecule incorporating just one oxygen atom in ninety carbon atoms, in close to monolayer coverage on Ag(111), which means an effective oxygen coverage of the order of 0.05 ML.

## 2. Experimental details

A sample of  $C_{60}Ph_5-OH$  in powder form was obtained from P. R. Birkett, Manchester, and prepared similarly to other phenylated  $C_{60}$  molecules [15]. It has had its (electronic) photophysical properties described elsewhere [16]. The molecule consists of a buckyball basis with five phenyl groups and one OH group attached to carbon atoms surrounding a central pentagon as depicted in Fig. 1 (see also Fig. 5 for a Schlegel diagram of the molecule). Preparation of  $C_{60}Ph_5-OH$  produces two isomers, in this paper, we concentrate on isomer I, which is the more symmetric and dominant one.

The addition of phenyl groups to the symmetrical  $C_{60}$  molecule significantly reduces the symmetry from  $I_h$  to pseudo- $C_s$  symmetry (isomer I) and alters the addend carbon atoms from being  $sp^2$  to  $sp^3$  hybridized, which has further consequences for the charge distribution along the cage [16]. Also, in contrast to  $C_{60}Ph_5-H$ , the OH group is not bonded to a carbon atom of the inner pentagon itself, but instead has exchanged places with one of the phenyl groups.

For the experiments the  $C_{60}Ph_5-OH$  powder was loaded in a Ta crucible of a K-cell mounted on a transfer arm. After thorough degassing in vacuum at around 300 °C, deposition lasted 30 min whilst the temperature was ramped slowly from 380 to 420 °C onto a clean Ag(111) surface.

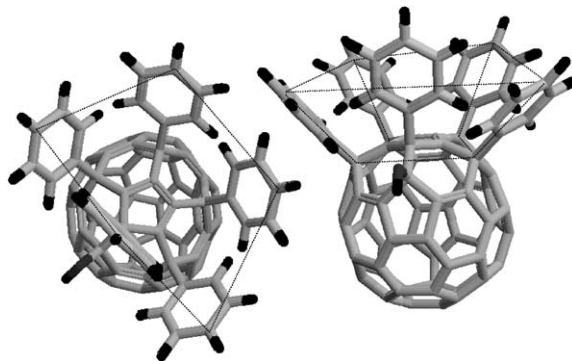


Fig. 1. Schematic, geometrically optimized diagram of  $C_{60}Ph_5-OH$  in top view and side view. The dotted lines indicate planes that we have used to simplify depiction of the molecule on the surface.

kept at 330 °C degrees allowing the molecule to diffuse and rotate freely to optimize its configuration on the surface and this also ensures that the coverage does not exceed a monolayer. The K-cell transfer arm construction allowed us to bring the crucible up to just 1 cm away from the sample and was used as the deposition rate of these phenylated molecules is very low in normal configurations (0.5 ML/h) [17]. Raising the deposition temperature is unfortunately not possible as the molecule is prone to disintegrate, which manifests itself by way of a colour change of the powder: from bright orange to a dull rust-brown, becoming darker as the temperature becomes higher. We, therefore, compared the remnants in the crucible after the experiment with unused molecules to verify that the chemical composition had not been altered in deposition. The base pressure of the UHV chamber was  $1.5 \times 10^{-10}$  Torr and rose to  $5 \times 10^{-9}$  Torr during deposition. C 1s and O 1s core level measurements were performed at 2.61 keV directly after deposition and revealed a ratio of C:O of  $\approx 100:1$ , after corrections using theoretical estimates for the cross-section [18].

NIXSW measurements were carried out at room temperature on beamline ID32 at the ESRF using a standard ultra-high vacuum (UHV) surface science chamber. The spectra were recorded using a hemispherical analyser (Physical Electronics) positioned at 45° to the incoming light provided by a double crystal monochromator. The substrate, a single crystal of Ag(111), was cleaned in UHV using standard argon ion sputtering and thermal annealing cycles of 550 °C and checked using X-ray photoelectron spectroscopy. Structural quality of the crystal was assessed using low energy electron diffraction (LEED) and NIXSW measurements of the substrate's AgMNN Auger spectra. A sharp (1x1) LEED pattern with a low background indicated the presence of a good surface reconstruction while structural parameters of  $f_{co} = 0.84 \pm 0.09$   $D = 0.98 \pm 0.02$  from the (111) reflection indicated that the mosaicity of the crystal was acceptable. Adsorbate and substrate NIXSW spectra were recorded simultaneously.

The valence band and core level PES experiments were carried out on beamline 5U1 of the synchrotron radiation source (SRS), Daresbury,

UK. The beamline uses a monochromator which has a single 1200 l/mm grating covering the energy range 60–1000 eV. The emitted photoelectrons were measured using a single channel hemispherical analyser, which permitted an overall instrumental resolution varying between 0.25 eV at the lowest end to around 1.2 eV at the upper end of the energy range. The base pressure was  $2 \times 10^{-10}$  Torr and rose to  $6.5 \times 10^{-9}$  Torr during deposition. Sample preparation was carried out in a similar way.

### 3. Results

In order to characterize the molecule, we have measured the valence band (VB), C 1s, and O 1s spectra (Fig. 2). The valence band is quite different from that of pure C<sub>60</sub> [19], which is unsurprising since C<sub>60</sub>Ph<sub>5</sub>-OH has lower symmetry and includes phenyl and sp<sup>3</sup> carbon species. Although the effect of these phenyl groups is clearly strong, the visible peaks in the VB can still be linked to those in a pristine C<sub>60</sub> spectrum and the largest change is perhaps the partial loss of the highest occupied molecular orbital (HOMO) suggesting finite electron donation of the buckyball to the OH and phenyl groups. The spectrum resembles that of C<sub>60</sub>Ph<sub>5</sub>-H [20], which is corroborated by theoretical calculations of the HOMO and the lowest unoccupied molecular orbital (LUMO), that show that both these low-lying energy levels are entirely located on the buckyball [21].

The C 1s spectrum shows a peak much wider (FWHM = 1.35 eV) than that of C<sub>60</sub> (FWHM around 0.4 eV) and consists indeed of at least three components. The small structure around 291 eV is identified as the  $\pi$ -electron plasmon. The O 1s is very weak, and has a tail towards higher binding energies, which indicates significant loss processes encountered by the photo-electron on its way out to the surface [22]. The C:O ratio found in these spectra after beamline and cross-section [23] correction is 115:1, instead of 90:1. The excess carbon could still be caused by some fraction of the molecules disintegrating during deposition, and the temperature during deposition for the

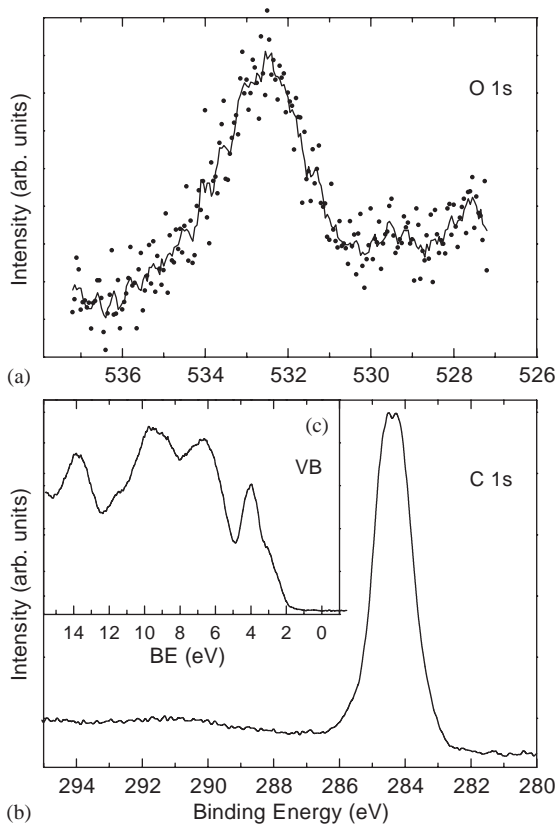


Fig. 2. (a) O 1s core level spectra taken at a photon energy  $E_{ph} = 850$  eV on a thin (ML) film of  $C_{60}Ph_5-OH$ , (b) C 1s spectra taken at  $E_{ph} = 350$  eV on the same film. (c) Valence band spectra taken at  $E_{ph} = 60$  eV taken on a thick film.

XSW experiment was therefore kept  $20^\circ$  lower at  $420^\circ C$ .

We have used an elaborate measuring and fitting procedure for our NIXSW experiment, which will be explained here. The O 1s spectra throughout the Bragg energy range were recorded over an interval large enough to allow inclusion of sufficient background points (Fig. 3a). This was deemed necessary as the O 1s signal is only marginally larger than the noise level in some areas of the energy range. This, combined with a 5–7 s counting time per spectrum point (compared to 0.1 s for the silver control signal), allowed us to separate the oxygen from the background signal. This is adamant, as the intensity profile traced out by the background signal could dominate that of the

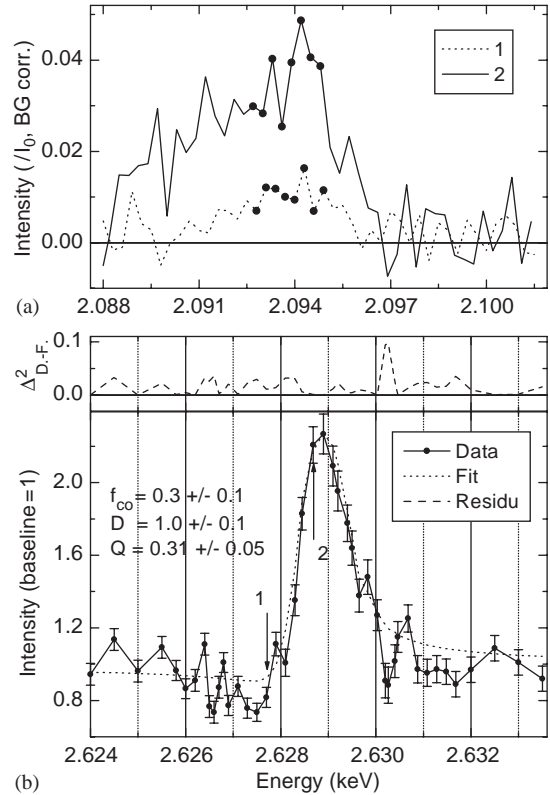


Fig. 3. (a) Examples of measured oxygen signals at photon energy positions indicated in bottom graph. The dots represent the data points used to construct the XSW yield points in b) as explained in the text. (b) Constructed XSW yield data points, fit and residue.

weak oxygen signal, resulting in a profile with a  $f_{co}$  and  $D$  which effectively trace those of the silver substrate. In our spectra, however, even though we find a value for  $D$  of  $2.35 \text{ \AA} = d_{Ag}$  which could be an indication of background interference, no reasonable fit could be achieved with a  $Q$  value around 0 (Auger like source), and only values around  $Q = 0.31$  gave the right profile, consistent with the PTCDA value for the O 1s measured using the same set up [11].

We chose to break up the XSW measurement into 1 eV intervals for several reasons. Firstly, in case of sudden beam loss we would have a higher probability of having a rough outline of the profile. Secondly, to allow for different counting times on the O 1s peak when traversing the Bragg



energy: longer in the wings and dip area of the electron yield curve, where the O 1s intensity is expected to be small, and somewhat shorter in the peak area. Lastly, it allows the observation of any effects of radiation damage, as the same energy range was covered several times. This proved very important as Fig. 4b indeed shows clear evidence of signal decay: the solid lines represent the first round of measurements, the dashed line the next set, and the dotted lines the last one. Although all the 1 eV measurements follow each other in time nearly without stopping, and therefore the first, second and third round were measured directly after one another, the time period between two

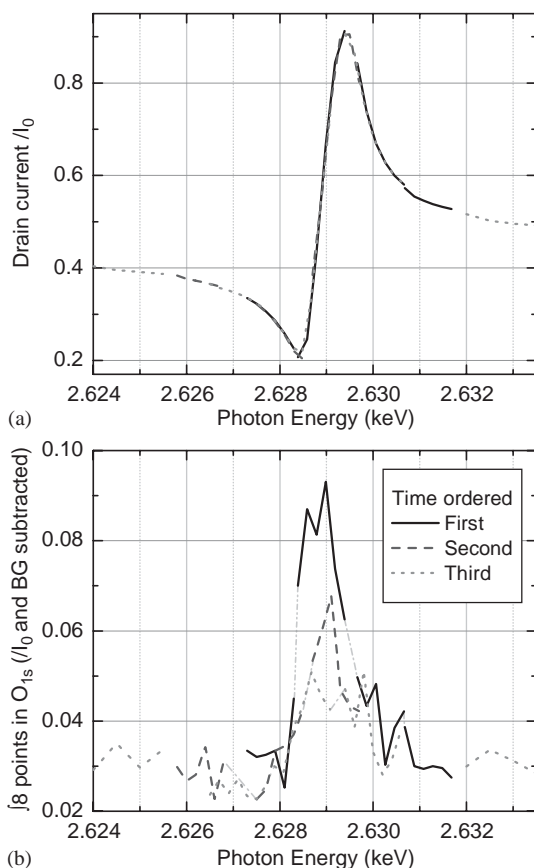


Fig. 4. (a) Drain current of the Ag(111) crystal used to align the O 1s XSW spectra depicted below. (b) Oxygen 1s yield curves for three successive XSW scans, obtained as explained in the text. Dash dotted lines connect successive measurements within one scan through the energy region.

“peak crossings” was approximately 2.5 h. Especially in this peak area the continuing decrease of signal in time is clear. This is not entirely surprising as we have found that the molecule is sensitive to temperature. Our study was performed at room-temperature, and sample cooling could offer a possible way of halting some of the disintegration process. Another solution for fragile samples is a “moving target” set up, but this would also be problematic as most Ag substrates are effectively a mosaic of differently oriented single crystals. One can see the “Catch 22” situation here: there is an obvious need for a 3rd generation light source of sufficient intensity and stability to allow for such demanding experiments, but on the other hand, the use of organic molecules brings with it a certain fragility and sensitivity to intense X-rays.

After corrections for beam-intensity, background and different time/point, we identified a region of just 8 points that was consistently “on” the O 1s peak in all spectra and summed only over this specific interval (see Fig. 3a). The resulting values were then brought together and aligned on the photon energy scale using the drain current measurement of the silver crystal. This is plotted in Fig. 4. In order to attempt a fit to this spectrum, we chose to average over the different sets, as none of them separately covers the entire Bragg range. The resulting spectrum and the fit are plotted in Fig. 3b. We can justify this as  $f_{co}$  is the main parameter that was influenced by the change in the central peak, which seems logical if the O 1s peak intensity and thereby the number of oxygen atoms decreases. We would like to emphasize again that this is just a preliminary study, but we will, however, offer an interpretation of the  $D$  value and its consequences for the orientation of the molecule. Using Arguslab [21] we constructed and optimized a model of the  $C_{60}Ph_5-OH$  molecule, and so obtained a measure for the size and angles (within 1% consistent with values quoted in [16]). At this point, we will just use the geometrical data for positioning the molecule and neglect any relaxation or bonding effects it might feel on the surface. Combining this model with the lattice spacing  $d = 2.35 \text{ \AA}$  of the Ag crystal resulted in three clear possibilities for the orientation of the

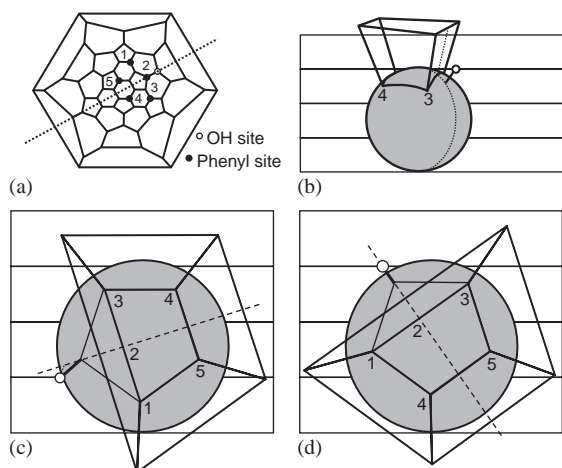


Fig. 5. (a) Schlegel diagram of  $C_{60}Ph_5-OH$ . (b–d) Possible orientations of  $C_{60}Ph_5-OH$  on the surface, consistent with  $D = 2.35\text{Å}$ .

molecule as summarized in Fig. 5b–d. Firstly, the molecule can sit with the phenyl arms pointing up, giving a distance of approximately  $D \approx 3d$  for the oxygen atom with respect to the surface (Fig. 5b). The other two possibilities have the molecule on its side, resting symmetrically on one phenyl group. In Fig. 5c the molecule rests on phenyl group 4 or 5 (see Schlegel diagram in a) for numbering), which are equivalent by symmetry, and this places the oxygen atom at  $D \approx 1d$  above the surface. The other sideways possibility lets phenyl group 1 or 3 rest on the surface, placing the O at  $D \approx 3d$  (Fig. 5).

Other orientations where the molecule rests on two groups, or where the molecule stands on all phenyl groups are not possible for this value of  $D$ . An orientation where the molecules rests on groups 1, 2 and 3, and effectively pushes the oxygen into the surface layer was discarded as it would put too much strain on the C–O bond. Lastly, “random” orientations in between the aforementioned positions (which were chosen because they comply with the symmetry of the molecule) were not taken into consideration. Using the three possibilities, however, a second NIXSW measurement at the  $(\bar{1}11)$  reflection could further distinguish between a height of around  $3d$  or  $1d$  above the surface, eliminating either (c) or both (b) and (d), whereas combination

with STM measurements can give an answer as to whether the molecule lies sideways or sits up. In  $C_{60}Ph_5-H$  the molecule is seen in STM to lie on its side with two phenyl legs pointing up [17], consistent with (c) and (d). The great similarity between photoelectron spectra of both these molecules, therefore, pushes us towards favouring the “sideways” orientation over the “upright” one.

#### 4. Conclusions

In conclusion, we have performed a “proof of principle” NIXSW experiment on low coverages of a low  $Z$  element (using the O 1s of  $C_{60}Ph_5-OH$  on  $Ag(111)$ ) and find the technique, employed using a 3rd generation light source, in principle able to cope with these extreme limits. We tentatively report a coherent fraction  $f_{co}$  of 30% and a coherent position  $D_{co}$  of  $2.35\text{Å}$ , and this is consistent with a molecule lying sideways and resting on a single phenyl group. We have, however, observed radiation damage effects manifested in loss of signal with time and a consequential loss in the coherent fraction. This does provide a further thinking point for the NIXSW technique if it is to be used for, often fragile, organic molecules.

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