

## Electronic structure of autoassembled TCNQ molecules deposited on Cu (100)

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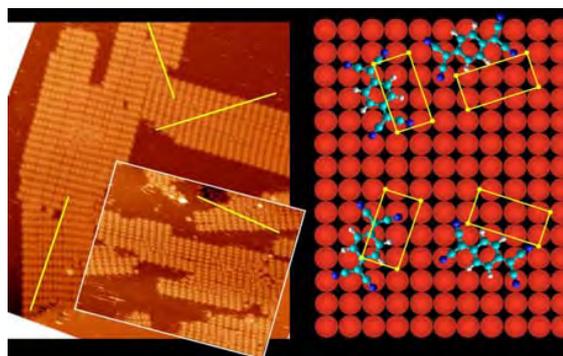
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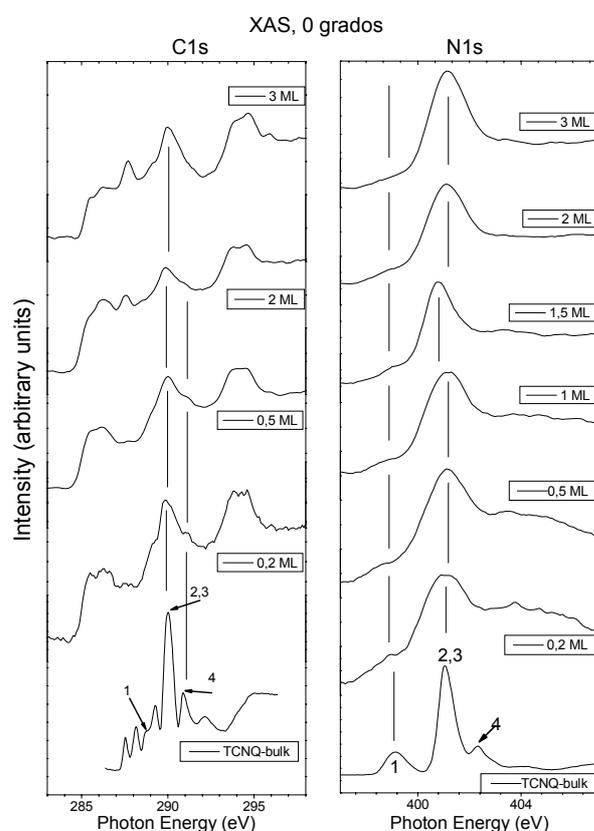
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The main purpose of this project is the study of the electronic structure of TCNQ organic molecules deposited on a clean Cu (100) surface. These molecules are characterized by their electronic properties, being electron acceptor.<sup>1</sup> It is known that when deposited on a Cu (100) surface, these molecules become autoassembled<sup>2</sup> (Fig.1) however the electronic interaction of these



**Fig. 1: STM images and orientation derived model of TCNQ/Cu (100).**



**Fig. 2: C 1s and N 1s XAS spectra at normal incidence as a function of the coverage**

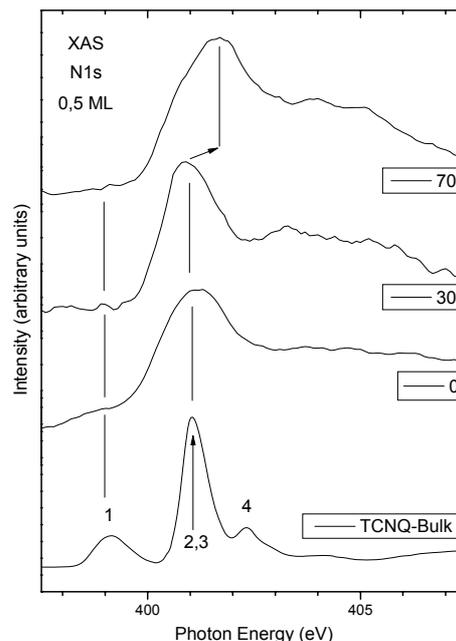
molecules with the substrate is an important topic that is not yet understood. We present preliminary results on this system obtained by X-ray absorption (XAS) and X-ray photoemission (PES) spectroscopies at the PM4 beamline at BESSY.

The C 1s x-ray absorption spectra at normal incidence of the TCNQ/Cu (100) surface as a function of the coverage are shown in Fig.2. The spectra are also compared to those obtained by Fraxedas et al<sup>3</sup> for bulk TCNQ. According to the assignments made by these authors, the main peak of both, C 1s and N 1s spectra, which are derived from the

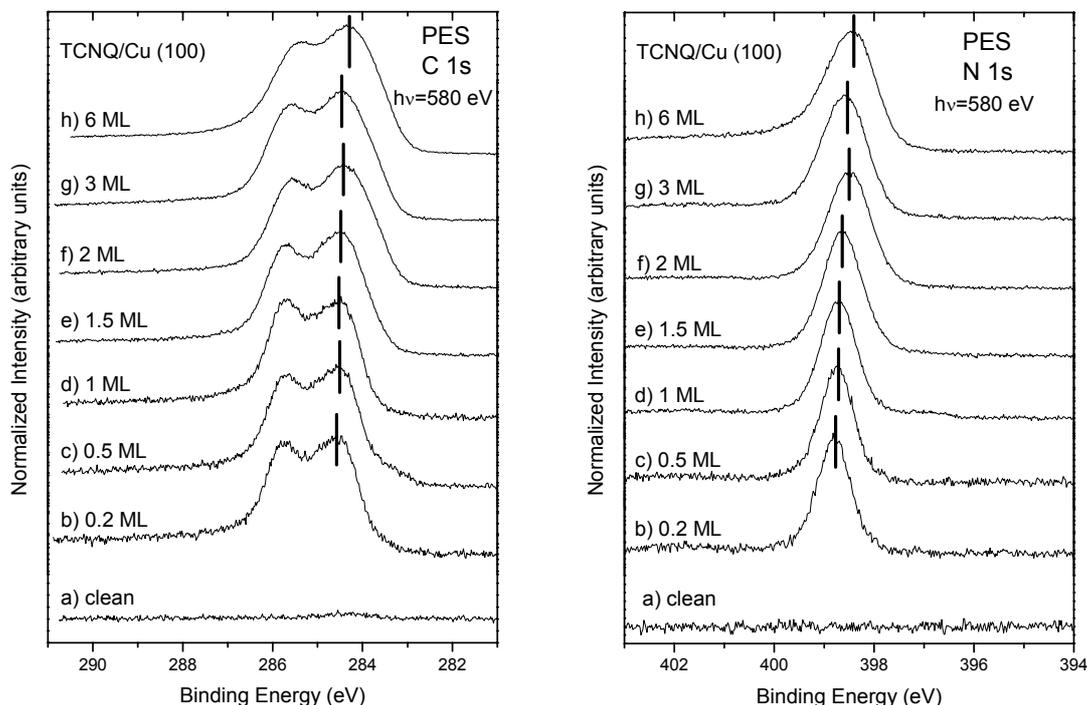
CN groups of the TCNQ molecule, are broadened with respect to those of the bulk molecule. This seems to indicate, as expected, a significant charge transfer from the Cu substrate to the TCNQ molecule.

This is also confirmed by angle dependent XAS spectra at the N 1s edge for a coverage of 0.5 ML shown in Fig. 3. Indeed, the broad peak assigned to the CN groups changes its intensity with the incidence angle. This is consistent with the splitting of these levels due to the charge transfer in the direction towards the Cu substrate.

The photoemission C1s and N 1s spectra of the TCNQ molecule as a function of the coverage are presented in Fig. 4. The spectra have been normalized for comparison purposes. For the C 1s



**Fig. 3: N 1s XAS spectra for 0.5 ML TCNQ/Cu (100) as a function of the incident angle**

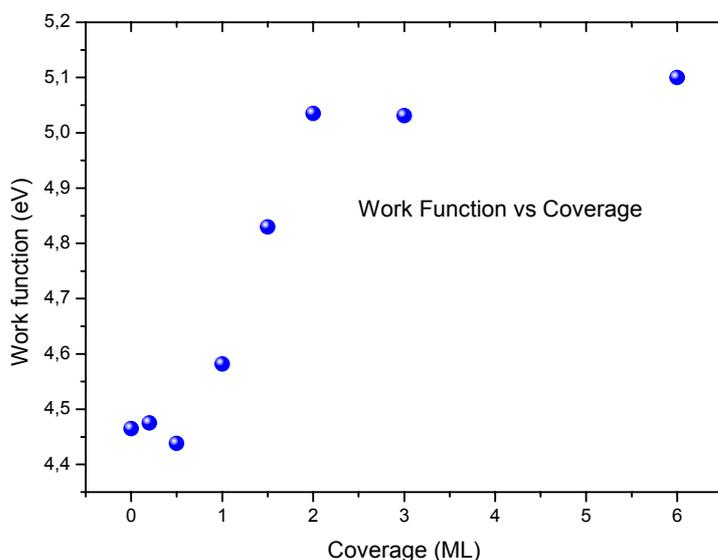


**Fig. 4: C 1s and N 1s photoemission spectra of TCNQ molecules deposited on a Cu (100) substrate as a function of the coverage**

spectra, they are formed by two different clearly observable peaks and a third peak hidden in between them. This agrees with the three different C atoms present in the TCNQ molecule,

i.e, benzoic ring, CN groups and intermediate C atoms. The higher binding energy peak, which is associated to the CN groups, is progressively shifting towards lower binding energies as the coverage increases. This is also consistent with the charge transfer produced from the Cu substrate to the CN groups. The above results are also corroborated by the N 1s XPS spectra shown in Fig.4. In this case, the spectra are formed by a single peak, as corresponds to the only N position in the TCNQ molecule. It can also be seen a similar shift towards lower binding energies of the peak as the coverage increases.

Finally, we have also measured the work function of the analyzed surface as a function of the coverage. The results are presented in Fig. 5. As the coverage increases up to 2 ML, the work function increases linearly from 4.5 to 5.05 eV. Then it remains almost constant for further depositions. This is again in agreement with the charge transfer produced from the Cu substrate to the first monolayer. Further coverages do not produce any significant change of the work function indicating that upon addition of the upper TCNQ monolayers the molecules do not receive any extra charge from the substrate.



**Fig. 5: Work function of the TCNQ/Cu (100) surface as a function of the TCNQ coverage.**

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**References:**

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