

## Electronic structure of Ex-TTF molecules deposited on Au (111)

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The main purpose of this project is the study of the electronic structure of organic molecules (Extended TTF) deposited on a clean Au (111) surface. These molecules are characterized by their electronic properties, being electron donor.<sup>1</sup> The interaction of these molecules with the substrate is an important topic in the context of efficient organic solar cells<sup>2</sup> that is not yet understood. X-ray absorption (XAS) and X-ray photoemission (PES) spectroscopies should address this question giving their HOMO and LUMO orbitals as a function of the coverage.

In this report we present preliminary results on the photoemission spectra for

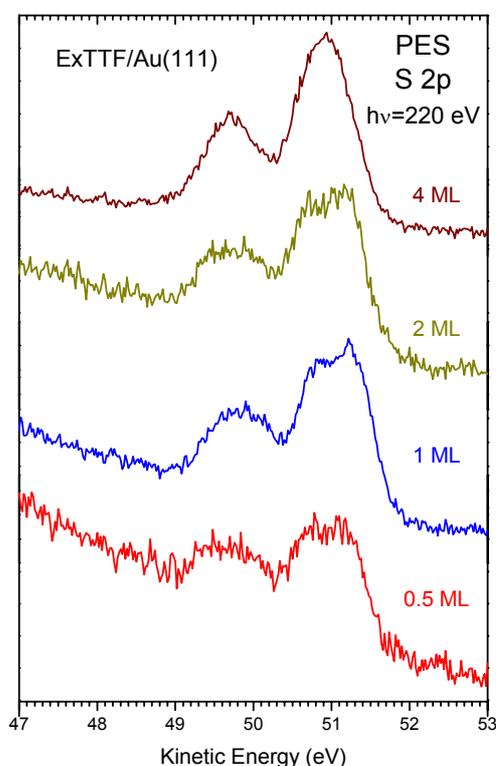


Fig. 1: S 2p photoemission spectra of the Ex-TTF molecules deposited on Au (111) as a function of the coverage

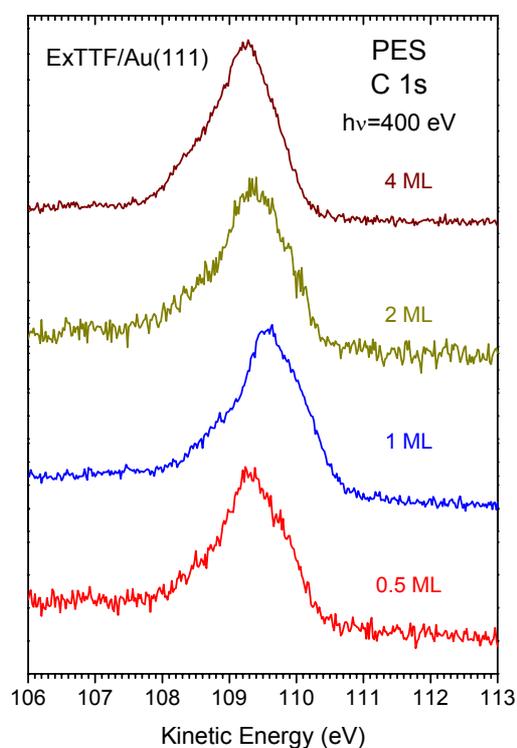


Fig. 2: C 1s photoemission spectra of the Ex-TTF molecules deposited on Au (111) as a function of the coverage

different coverages of Ex-TTF molecules deposited on clean Au (111). Fig.1 shows de photoemission S 2p spectra as a function of the coverage.

The spectra for low coverages (0.5, 1 and 2 ML) clearly show that each main peak of the 2p doublet in the S 2p spectra is formed by two peaks, thus indicating that two different S atomic positions are observed in the spectra. This is in good agreement with previous theoretical calculation on the predicted Ex-TTF molecule arrangement on a Au (111) surface,<sup>3</sup> in which two of the four S atoms of the molecule are in direct contact with the Au (111) surface whereas the other two S atoms remain upwards (see Fig.3). On the other hand, the spectrum

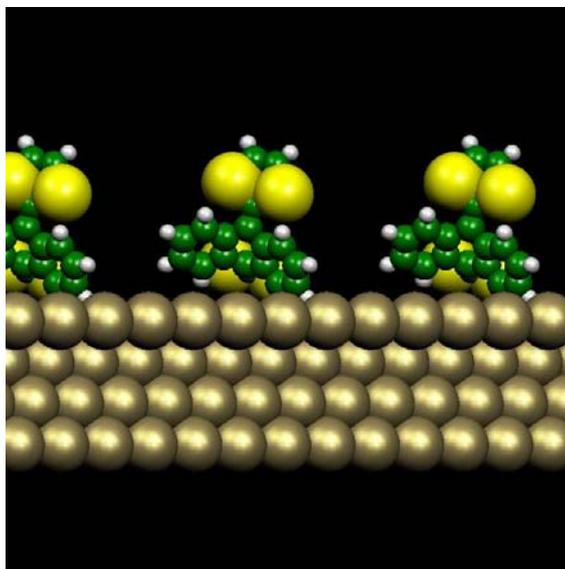


Fig. 3 Spatial representation of the calculations for an Ex-TTF molecule adsorbed on a Au (111) surface

corresponding to 4 ML of molecules deposited on the Au (111) surface shows a narrower peak indicating that only one equivalent atomic position for S atoms dominates the spectrum, in agreement with the theoretical model.

The C 1s photoemission spectra of the Ex-TTF molecule on the Au (111) surface are shown in Fig.2. The spectra show a rather complex and asymmetric peak which is clearly formed by different contributions, reflecting the different environment of the C atoms in the Ex-TTF molecule. In order to obtain more information from these spectra a more detailed analysis is needed. However the similarity of the spectra throughout the series seems to indicate that C atoms are less affected by the interaction with the substrate.

#### References:

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