

Supporting information.

Thiophene Derivatives on Gold and Molecular Dissociation Processes

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Contents:

1. Au 4f spectra for clean Au(111) and after thiophene adsorption.
2. Overview spectra
3. A different 3T adsorption XPS spectrum and corresponding NEXAFS data for a case with dissociation.
4. Damage evolution for 1T and 3T at the TEMPO beamline
5. Variability: spectra for several samples for the same molecule.

Au4f spectra.

Spectra in the Au 4f region measured at the TEMPO beamline for pristine Au(111) and after thiophene adsorption are shown in Figure S1. For the pristine surface the spectrum displays the characteristic low energy shoulder due to Au surface atoms. This feature disappears upon adsorption as is well known for chemisorption of other thiols.

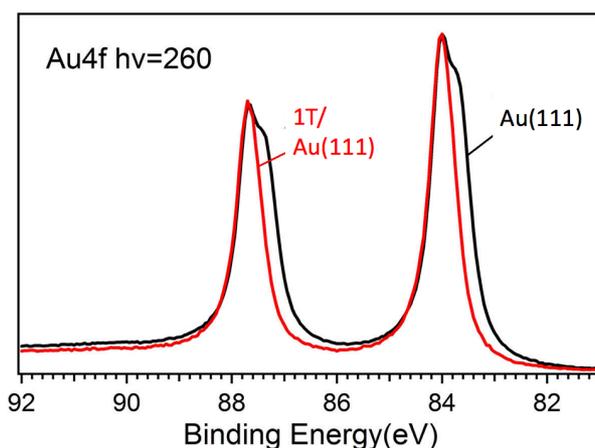


Figure S1. Comparison of Au4f_{7/2} spectral line shape (normalized) for the Au(111) monocrystal before and after thiophene adsorption.

Overview Spectra.

Overview spectra for adsorption of some molecules on the gold on mica substrates and on the Au(111) monocrystal. In case of the Au/Mica substrate these were taken on the $K\alpha$ spectrometer using the Al anode with 1486,6 eV photons. Some oxygen presence may be noted because of the use of solution processing and passage through air. Carbon presence is clear, however at this photon energy the S 2p signal is weak.

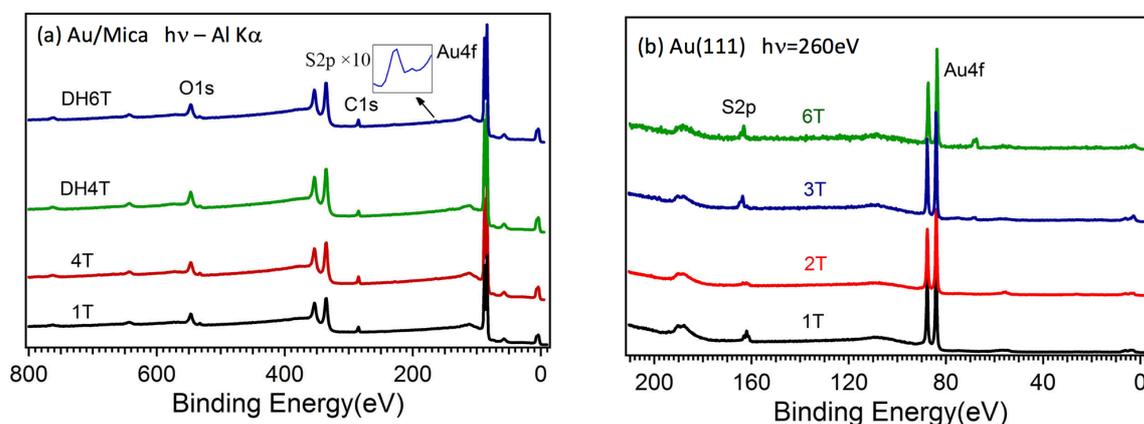


Figure S2 Overview spectra for adsorption of some thiophene molecules on (a) gold on mica substrates and (b) Au(111) sample.

Spectra for 3T

Figure S4 shows XPS and NEXAFS spectra for a different case of 3T adsorption on Au(111), where we see more intense 161 and 162 eV components and a broadened main peak indicating some dissociation occurred. In this case the NEXAFS spectra do not display a very strong peak at 285 eV due to the thiophene π^* resonance and no clear angular dependence is observed.

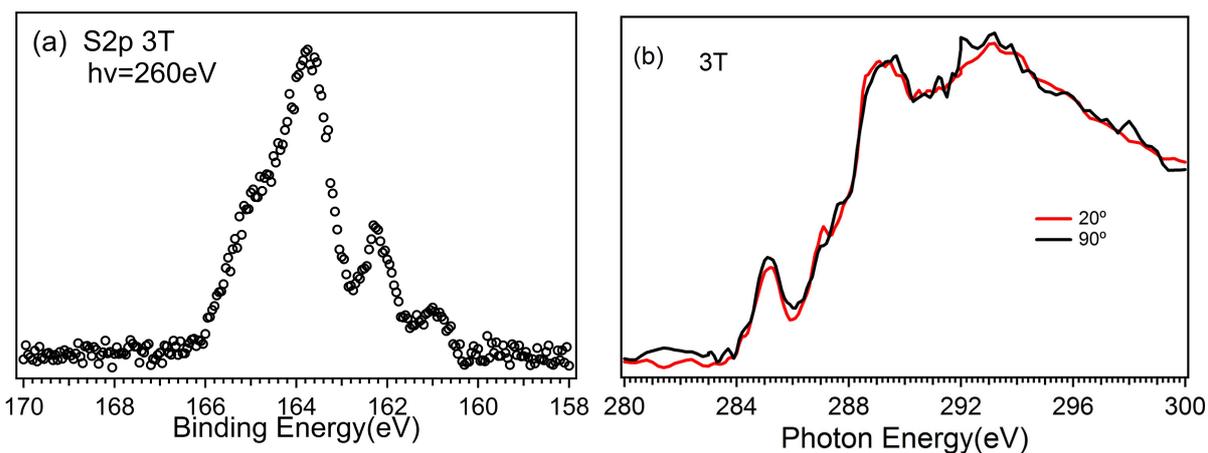


Figure S3. S2p spectrum of a 3T thiophene sample with larger A, B and D components and the corresponding C 1s NEXAFS spectrum.

X ray induced damage.

Color maps of intensities in the S 2p XPS spectra acquired scan by scan corresponding to the spectra in Figure 6 of the main text.

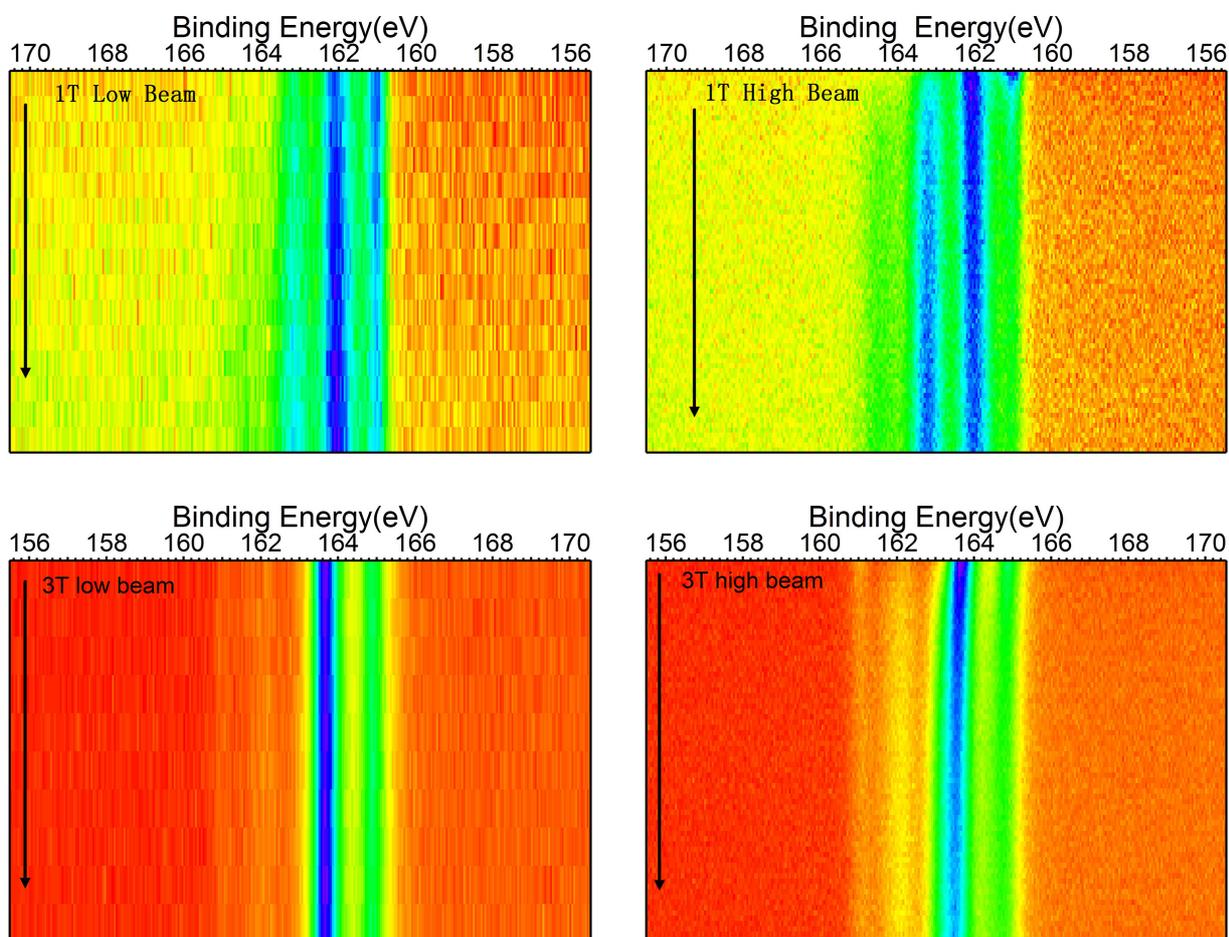


Figure S4. Color maps of the intensity in S2p spectra as a function of scanning for low intensity and high intensity beams for 1T and 3T. In the upper row (1T) the low beam image corresponds to 15 scans and the high beam one to 77 scans. In the lower row (3T) the low beam image corresponds to 10 scans and the high beam one to 72 scans.

Spectral variations.

In Figure S5 we show series of S2p spectra for adsorption of different thiophenes on the Au on mica substrates. The substrate, thiophene solution and SAM preparation procedures were the same. While the sample preparation procedures were the same one can observe variations in the shape of the spectra that are attributed to more or less significant presence of dissociation processes.

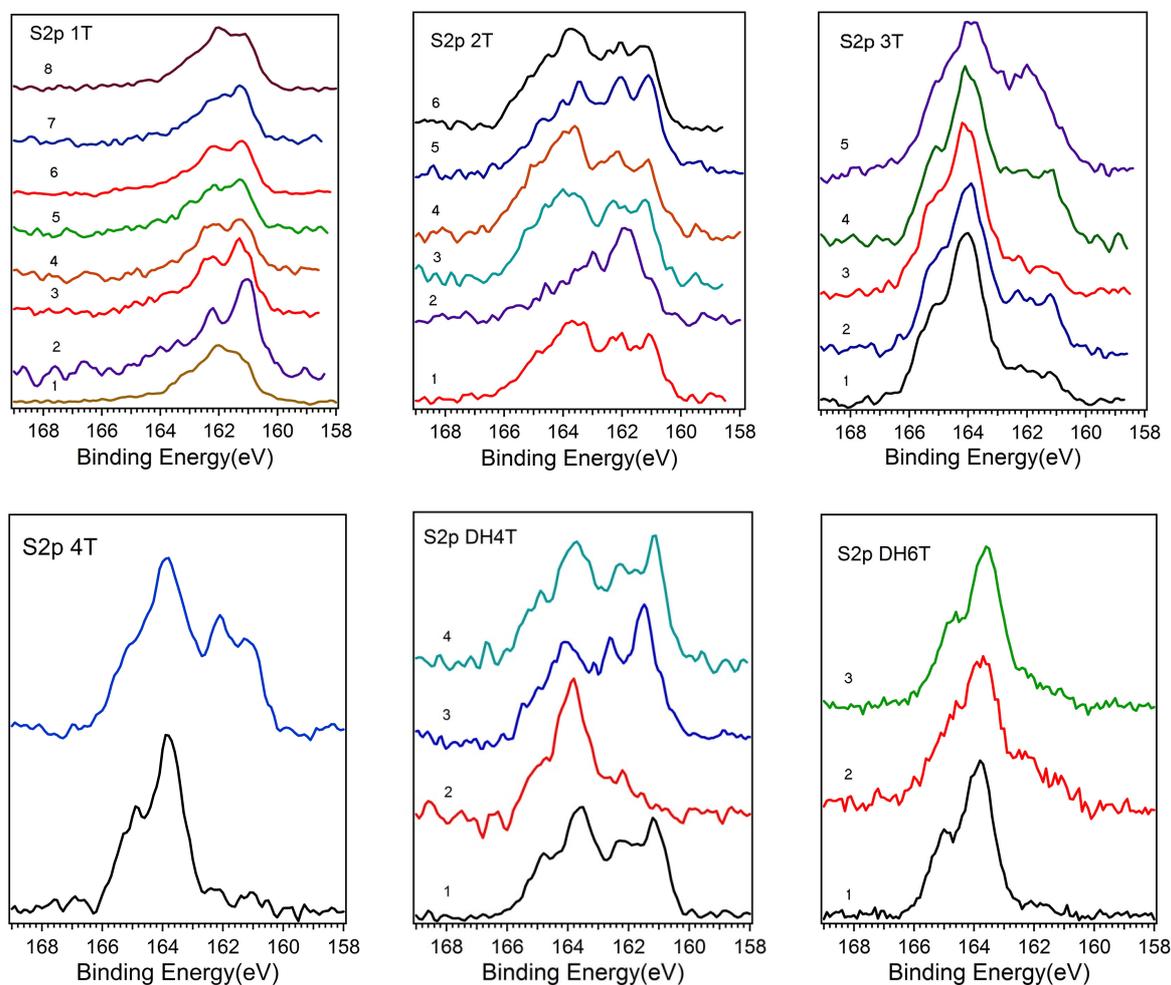


Figure S5. Variations in the S2p spectra of thiophene and derivative molecules obtained on different gold on mica samples following the same preparation procedures.