

ELECTRONIC SUPPORTING INFORMATION

# Thin Film Properties and Stability of a Potential Molecular Quantum Bit Based on Copper(II)

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This Supporting Information contains:

- 1) Stoichiometry and integrated XPS experimental signal intensities for the  $\text{Cu}(\text{dbm})_2$  thin films.
- 2) Fit results for the energy positions and relative intensities of the photoemission lines in the C1s spectra.
- 3) Air exposure stability after 10 weeks.
- 4) Supporting Information references.

1) Table S1. Stoichiometry and integrated XPS experimental signal intensities for the Cu(dbm)<sub>2</sub> thin films deposited on Au(110) single crystals.

	Stoichiometric composition	XPS Relative Intensity (%)	
		Thinnest film (4 Å)	Thickest film (105 Å)
C	86%	86%	84%
O	11%	11%	11%
Cu	3%	3%	3%

The sensitivity factors are:  $\sigma_{C1s} = 0.25$ ,  $\sigma_{O1s} = 0.66$   $\sigma_{Cu2p} = 6.3$ .<sup>1</sup>

2) Fit results for the energy positions and relative intensities of the photoemission lines in the C1s spectra.

Table S2. Fit results for the C1s contributions: thick films.

	<b>Energy</b>	<b>Lorentzian</b>	<b>Gaussian</b>	<b>Intensity</b>
	<b>(eV)</b>	<b>Width (eV)</b>	<b>Width (eV)</b>	<b>(%)</b>
C-C	284.1	0.08	0.85	12.0
C-H	284.9	0.08	0.85	71.1
S <sub>1</sub>	285.6	0.08	0.85	4.4
C-O	287.0	0.08	0.85	9.8
S <sub>2</sub>	291.3	0.08	1.90	2.6

Table S3. Fit results for the C1s contributions: monolayer.

	<b>Energy</b>	<b>Lorentzian</b>	<b>Gaussian</b>	<b>Intensity<sup>a</sup></b>
	<b>(eV)</b>	<b>Width (eV)</b>	<b>Width (eV)</b>	<b>(%)</b>
C-C	284.0	0.08	0.85	12.0
C-H	284.8	0.08	0.85	69.9
S <sub>1</sub>	285.5	0.08	0.85	4.4
C-O	286.9	0.08	0.85	10.0
S <sub>2</sub>	291.2	0.08	2.80	3.7

The satellite structures are denoted with S<sub>i</sub>,  $i = 1, 2, \dots$

The expected stoichiometric values for the C 1s elemental analysis are:

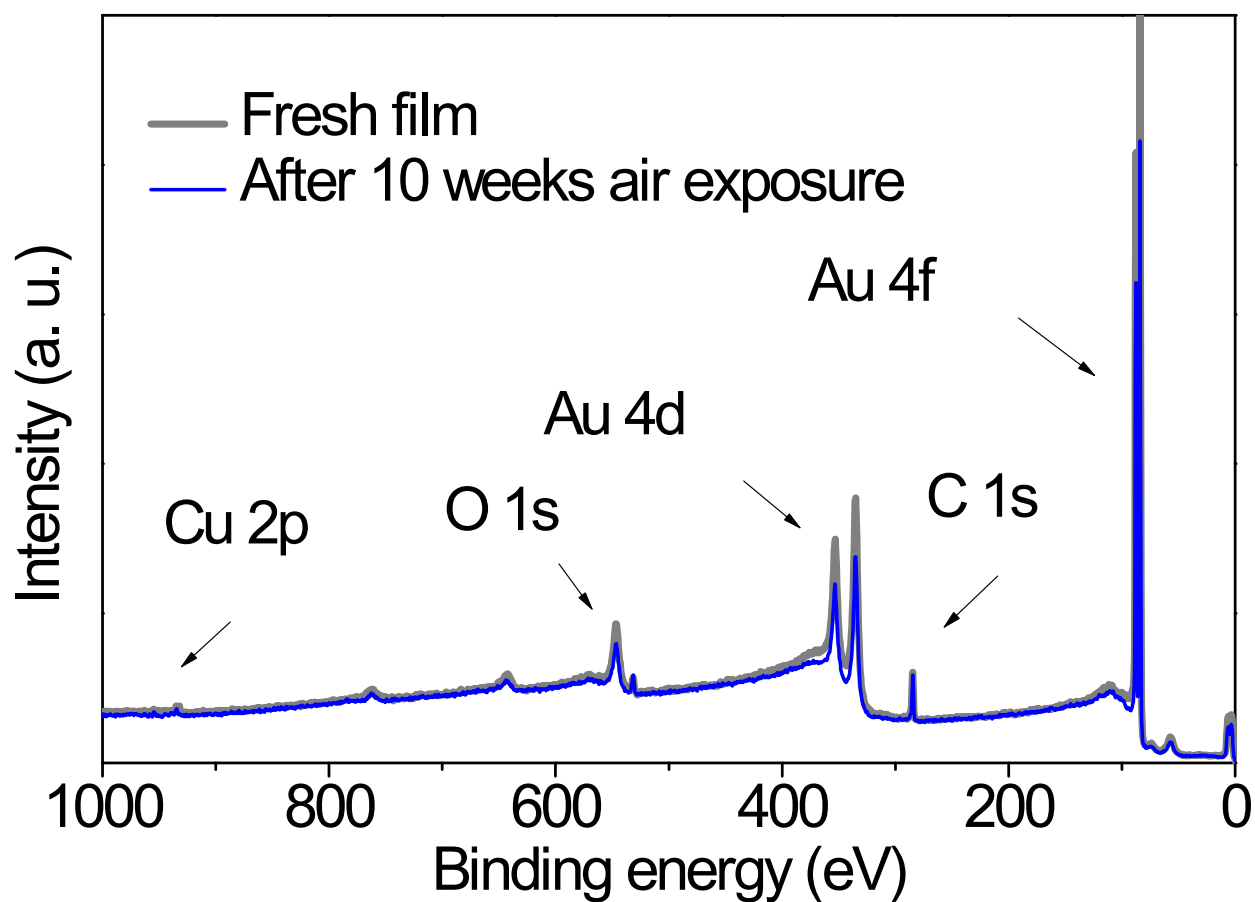
C-C = 13.3%

C-H = 73.3%

C-O = 13.3%

Thus, the intensity ratio of the sum of the contributions to the C1s main line and the C-O line is set to be 86.6:13.3. Analogously, the contributions to the main line are set to have an intensity ratio 13.3:73.3:13.3 as in the molecule taking also the satellite intensities into account.

3) Air exposure stability after 10 weeks



**Figure S 1.** Comparison of the survey spectra after 10 weeks air exposure. There are several differences in the main lines, as well as in the background, indicating chemical and morphological changes.

## Supporting Information References

1. Wagner, C. D., Sensitivity Factors for Xps Analysis of Surface Atoms. *J. Electron Spectrosc. Relat. Phenom.* **1983**, 32, 99-102.