

Supporting Information

for

The role of substrate commensurability in the surface-assisted synthesis of zigzag organometallic and oligophenylene chains

Jingya Dai¹, Qitang Fan¹, Tao Wang¹, Julian Kuttner², Gerhard Hilt², J. Michael Gottfried^{2*},
Junfa Zhu^{1*}

¹National Synchrotron Radiation Laboratory and Collaborative Innovation Center of Suzhou
Nano Science and Technology, University of Science and Technology of China, Hefei 230029,
P.R. China, jfzhu@ustc.edu.cn

²Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Str., 35032 Marburg,
Germany, michael.gottfried@chemie.uni-marburg.de

(a) XP spectrum of Br 3p after deposition of DMTP onto Cu(110) at 300 K

C-Br bonds of DMTP undergo cleavage on Cu(110) surface at 300 K. Evidence for this reaction is provided by the XP spectra in Figure S1. The blue curve shows the Br 3p XP spectra of DMTP, which was deposited onto the Cu(110) surface at 300 K. The Br 3p_{5/2} peak is located at 182.2 eV. This binding energy is 2.2 eV lower than that of Br in intact DMTP molecules on Cu(111).¹ This indicates that the chemical state of the Br atoms undergoes a dramatic change, which is attributed to the scission of C-Br bonds and the formation of a bromide like species.

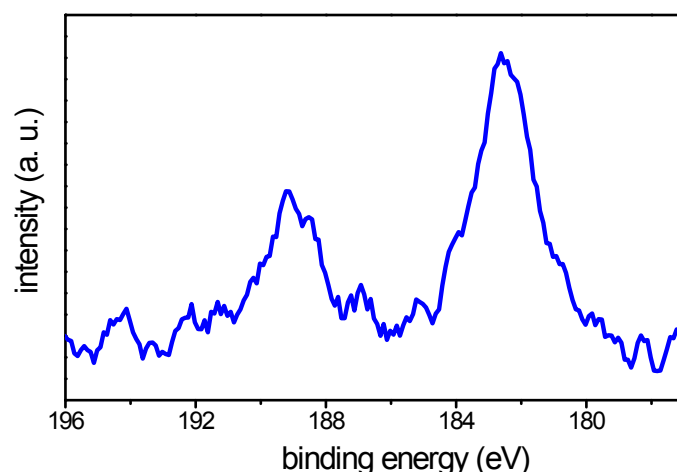


Figure S1. Br 3p XP spectra of 0.5 ML DMTP deposited onto Cu(110) at 300 K. XPS was performed with a VG MARK II spectrometer using a Mg K_α X-ray source ($h\nu=1253.6$ eV). The binding energies of Br 3p were referenced to the Fermi edge of clean Cu ($E_F \equiv 0$).

(b) Experimental and simulated LEED patterns

Figure S2 shows that the simulated LEED pattern corresponds well with the experimental LEED pattern.

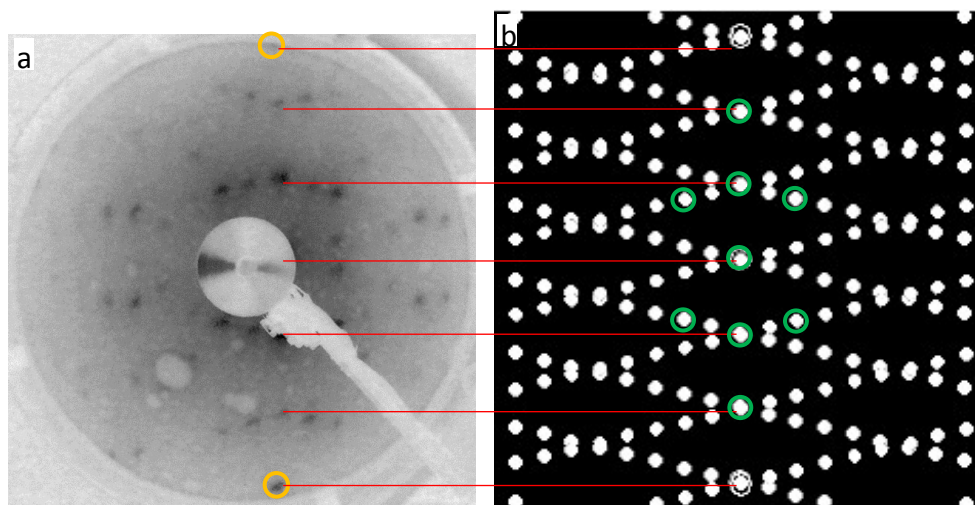


Figure S2. a) Experimental LEED pattern of the sample (0.84 ML DMTP deposit onto Cu(110) held at 383K). b) the simulated LEED pattern derived from the matrix of both $(3, 1 | 0, 11)$ and $(3, 10 | 0, 11)$.

References

1. Fan, Q.; Wang, C.; Liu, L.; Han, Y.; Zhao, J.; Zhu, J.; Kuttner, J.; Hilt, G.; Gottfried, J. M. Covalent, Organometallic, and Halogen-Bonded Nanomeshes from Tetrabromo-Terphenyl by Surface-Assisted Synthesis on Cu(111). *J.Phys. Chem. C* 2014, 118, 13018-13025.