A study on the heterostructures of CuPc on C_{60}/Ag(111) by LT-STM

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Introduction

Thin organic films of small-molecules have received an increasing attention in the past two decades due to the possible application for optical and electrical devices, such as OFET and Solar Cells. Controlling the complex interactions and the microstructure at the electrode-organic and organic-organic interfaces would support the optimization of such devices performance and improve their characteristics by lowering operating voltages and enhancing thermal stability. Here, the heterostructures between Copper Phthaloyanine (CuPc) and C_{60}, which were widely used in Solar Cells, were investigated using Low Temperature Scanning Tunneling Microscopy (LT-STM) and angle-dependent NEXAFS.

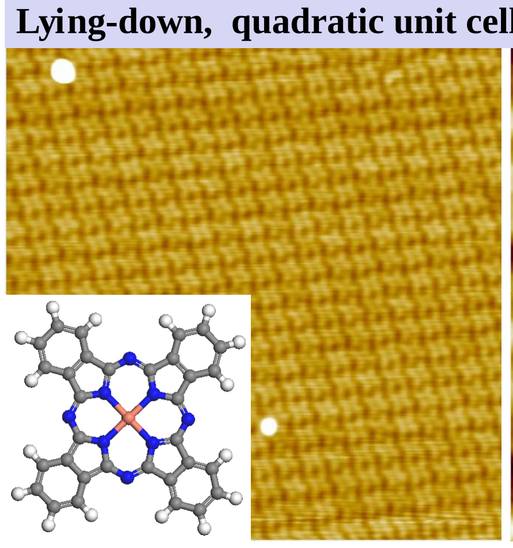
Experiment

- C_{60} and CuPc molecules were deposited from different K-cells, successively, onto a Ag(111) substrate at room temperature (RT) in UHV chamber.
- All the STM measurements were carried out by an Omicron low temperature scanning tunneling microscope at 77 K .
- The Angle-dependent N K-edge NEXAFS measurements were performed at the SINS beamline of the Singapore Synchrotron Light Source in total electron yield mode with a photon energy resolution of 0.1 eV at RT.

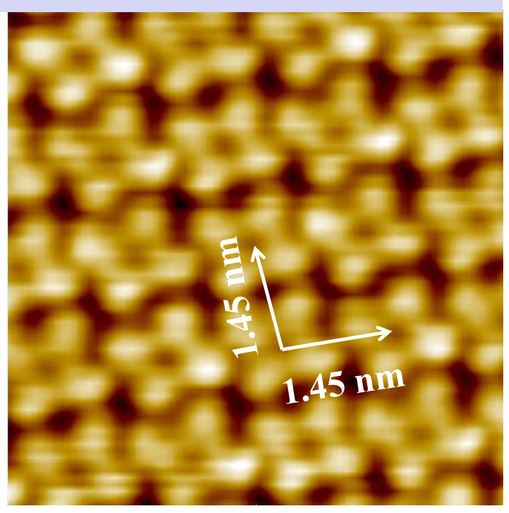
Results and Discussions

a) monolayer CuPc on Ag(111)

Lying-down, quadratic unit cells



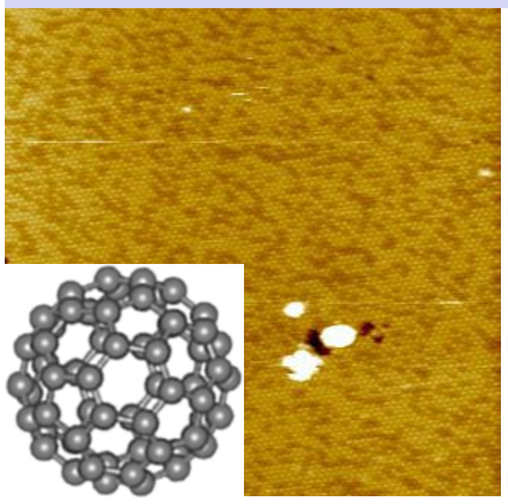
30 nm x 30 nm V_T= 0.8v



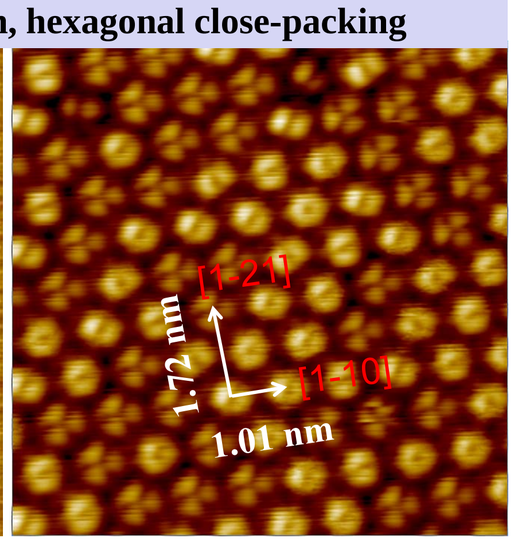
7 nm x 7 nm V_T=0.2 V

b) monolayer C_{60} on Ag(111)

Different molecular orientation, hexagonal close-packing



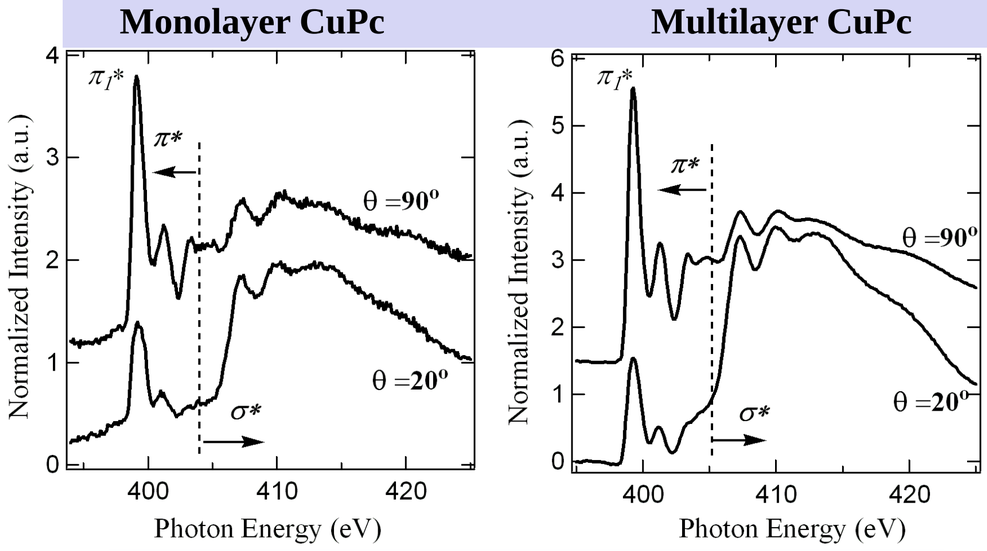
80 nm x 80 nm V_T=-2.4 V



10 nm x 10 nm V_T=-2.0 V

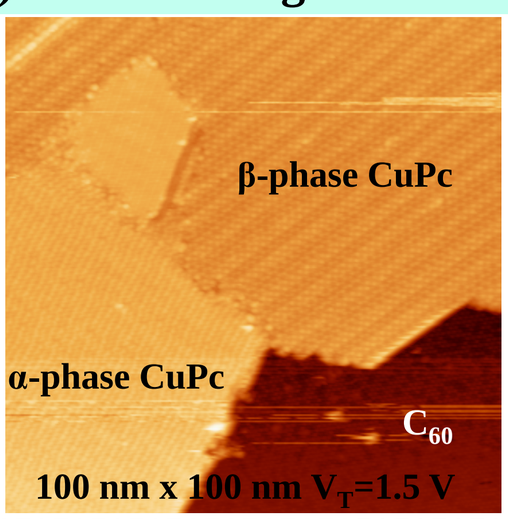
c) Angle-dependent N K-edge NEXAFS of CuPc on C_{60}/Ag(111)

Monolayer CuPc | Multilayer CuPc

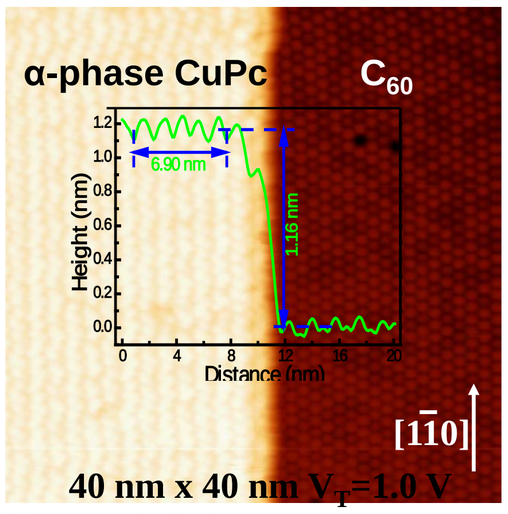


The CuPc molecular plane is tilted to the surface.

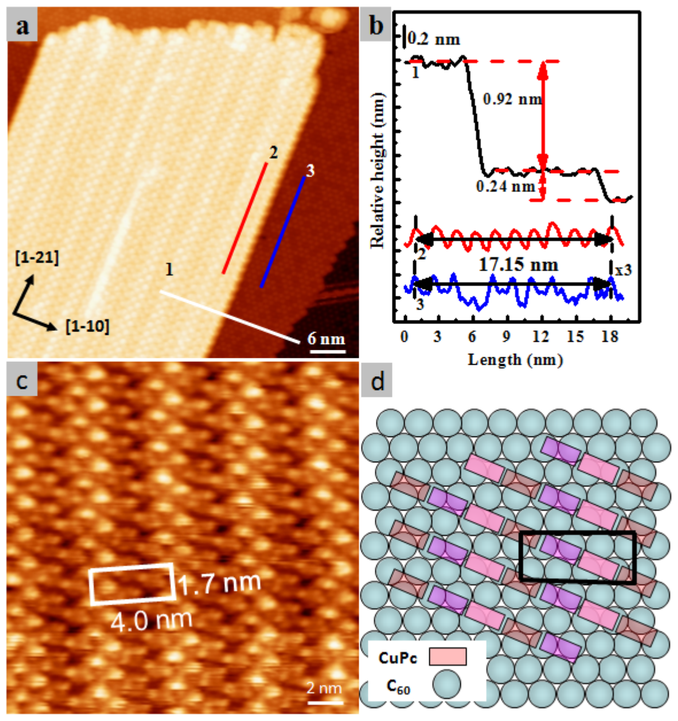
d) STM investigations:



~0.5 ML CuPc on C_{60}/Ag(111), two kinds of heterostructures are formed with an angle of 30° relative to each other, labeled as α-phase and β-phase, respectively.



STM image shows poor ordered α-phase CuPc molecular rows (the left half) along the [1-10] azimuth of hcp C_{60} monolayer (the right half). In the molecular rows, CuPc molecules arranged rather disordered. The inserted line profile reveals that the CuPc layer is around 1.16nm high and about 1.4nm wide, indicating that the CuPc molecules are not oriented parallel to the substrate.



a) STM image of pure β-phase CuPc on C_{60}/Ag(111) runing along along the[1-21] direction of hcp C_{60} ; b) line profiles show β-phase CuPc with a height of 0.92 nm and a width of 1.72 nm; c) corresponding close-up showing the moiré pattern with dimensions of 4 nm and 1.7 nm, the (4 x 1) unit cell containing 3 CuPc and 4 C_{60} molecules; revealing a commensurate epitaxy; d) schematic of proposed model.

Conclusions

- Upon deposition ~0.5 ML CuPc on C_{60}/Ag(111), two kinds of heterostructures are formed with an angle of 30° relative to each other. While one is in poor ordering, the other one is commensurate.
- The CuPc is tilted to the surface, proposed to be mainly determined through the attractive C-H···π electrostatic intermolecular interaction between CuPc and the underlying C_{60}。
- A model of the epitaxial CuPc on C_{60}/Ag(111) was proposed.