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
  - 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 1.16 nm high and about 1.4 nm wide, indicating that the CuPc molecules are not oriented parallel to the substrate.

- **b)** monolayer C_{60} on Ag(111)
  - Different molecular orientation, hexagonal close-packing
  - 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 1.16 nm high and about 1.4 nm wide, indicating that the CuPc molecules are not oriented parallel to the substrate.

- **c)** Angle-dependent N K-edge NEXAFS of CuPc on C_{60}/Ag(111)
  - The CuPc molecular plane is tilted to the surface.

- **d)** STM investigations:
  - 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 1.16 nm high and about 1.4 nm wide, indicating that the CuPc molecules are not oriented parallel to the substrate.

**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, labeled as α-phase and β-phase, respectively.
- 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.