

# Shielding Copper Atoms by Distortion of Phthalocyanine Ring on Si(111)

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## Introduction

- Metal phthalocyanines have attracted wide attentions as potential candidates in molecular electronic devices, i. e. light emitting diodes, laser diode, solar cell and gas sensors [1].
- Interfacial properties including molecule-substrate interactions and their effects on the electronic structure of the molecular layer remain be an interesting topic.

## Experimental

CuPc molecules were evaporated onto pre-cleaned Si(111)-(7x7) surface in UHV condition. One monolayer of CuPc on Si(111) surface was achieved by building up a thick, bulk-like layer of CuPc followed by an anneal at 300 °C

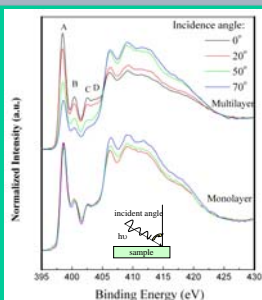


Schematic structure of CuPc molecule

Photoemission and X-ray absorption measurements were performed in Surface, Interface and Nanostructure Science (SINS) beamline, Singapore Synchrotron Light Source [2].

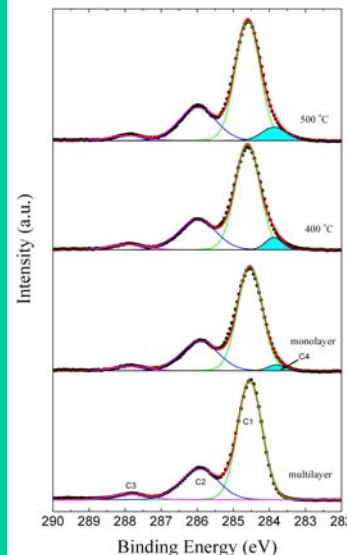
## Main Results

### I. X-ray absorption spectra (XAS) for multilayer and monolayer of CuPc



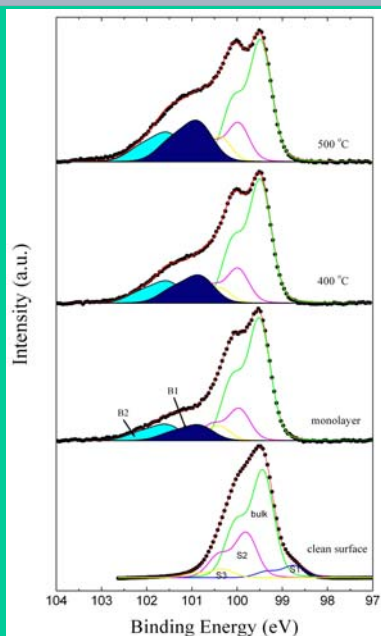
Molecular orientation for monolayer of CuPc is disordered in contrast to ordered orientation for a multilayer.

### III. C 1s core level spectra for multilayer of CuPc monolayer of CuPc and after post-annealing.



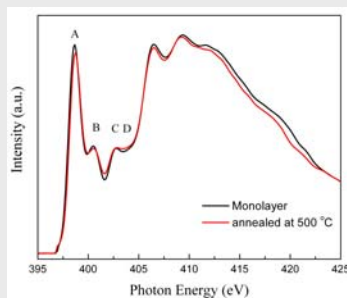
The presence of the component C4 reveals the formation of Si-C bonds between the molecules and the substrate and strong interaction of the substrate on the molecules. The remaining of the shakeup feature (C3) confirms that the molecular structure is not destroyed while the molecules are distorted.

### II. Si 2p core level spectra for clean Si(111)-(7x7), monolayer of CuPc on Si(111) and after post-annealing



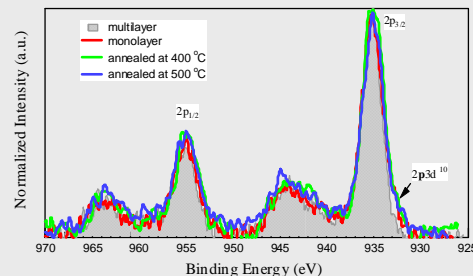
The component S1 related to the rest atoms in the (7x7) reconstruction completely disappeared after the adsorption of CuPc. Two components B1 and B2 emerge at high binding energy side, indicating the formation of bonding between the molecules and the Si surface

### IV. N K-edge XAS spectra before and after post-annealing.



The comparisons of the XAS spectra for monolayer of CuPc before and after annealing further confirms the integrity of the CuPc molecules.

### V. Cu 2p core level spectra for multilayer, monolayer of CuPc and after post annealing



A component corresponding to a  $2p3d^{10}$  final state (at 933 eV) reveals that some metal sites where the atom has the  $3d^{10}$  ground state are present in one monolayer of CuPc adsorbed on the Si(111) surface[3]. The valence state of the Cu atom remains the same as that for one monolayer of CuPc even after post-annealing at 500 °C.

## Conclusions

- Strong interaction between CuPc molecules and the Si(111) surface by formation of Si-C and Si-N bonds.
- Reduction of the valence state of the Cu atom from +2 to +1 is induced by Si-Cu interaction.
- The Cu atoms are well shielded by distortion of phthalocyanine ring in CuPc molecules on the Si(111) surface.

## References

- [1] F. H. Moser, Phthalocyanine Research and Application, CRC, Boca Ration, 1990; [2] X. Yu et al., J. Electron. Relat. Phenom 144, 1031 (2005); [3]G. Dufour et al., Surf. Sci. 319, 251 (1994)