

# Investigation of interface properties of DIP/F16CuPc heterojunctions: interface morphology, molecular orientation, energy level alignment

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## Introduction

Interface properties at organic-organic heterojunctions (OOHs) play important roles in organic electronics, such as organic solar cells, organic light emitting diodes and so on. Intensive research has been devoted to the investigation and understanding these interface properties, such as molecular orientation, energy level alignment, charge transfer dynamics.

In this work, in situ UPS, XPS and synchrotron based photoelectron spectroscopy (PES) and near-edge x-ray absorption fine structure (NEXAFS) measurements have been used to investigate the interface properties at the OOH comprising diindenoperylene (DIP) on both standing-up and lying-down copper-hexadecafluoro phthalocyanine (F16CuPc).

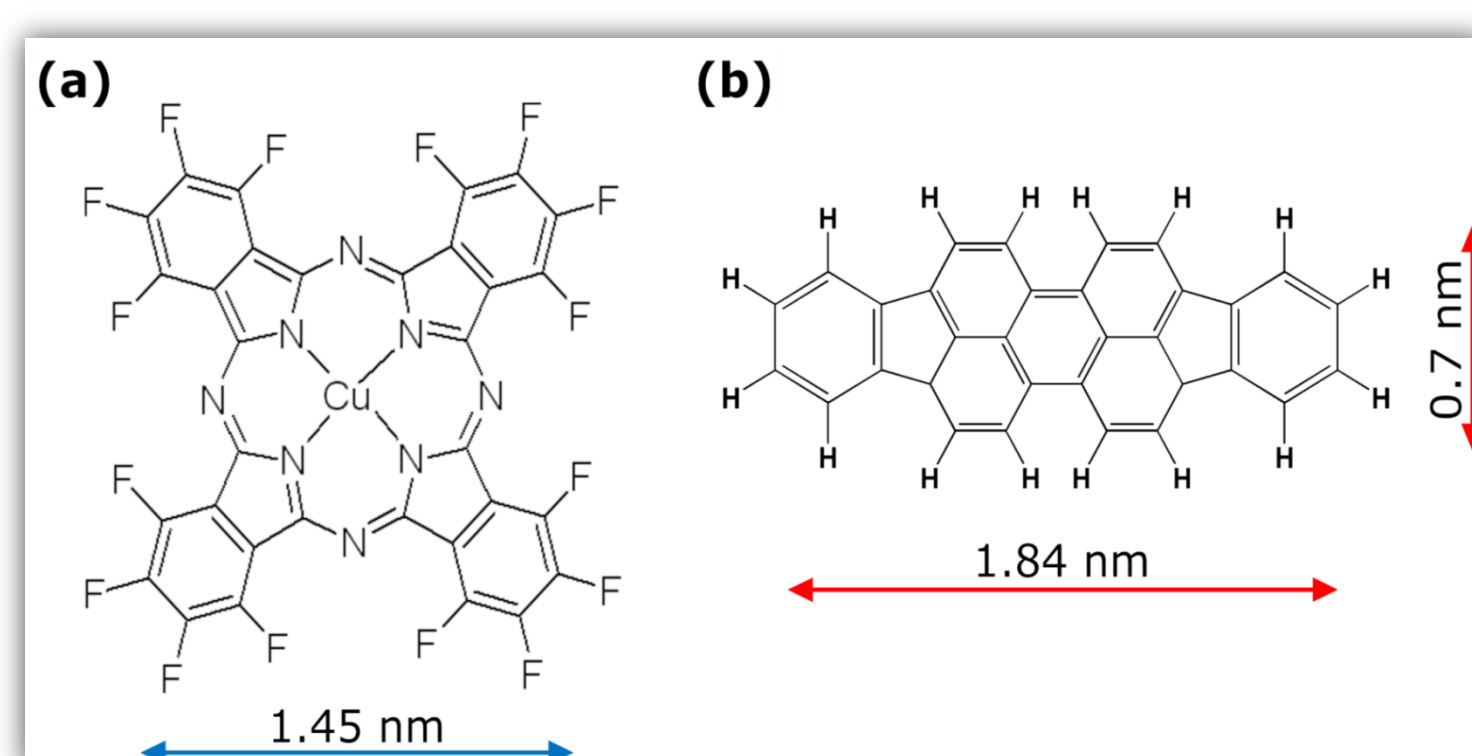


Fig1. Molecular structure of (a) F16CuPc and (b) DIP

## Methodology

In situ UPS and XPS measurements were carried out for the F16CuPc/DIP heterojunction on Si(111) with native oxide, and on highly oriented pyrolytic graphite (HOPG).

1. UPS measurements were performed with He 1 (21.2eV) as excitation source, a -5V bias was applied to the sample to allow the collection of the low kinetic energy part.
2. XPS studies were conducted with Al K $\alpha$  source at 1486.6eV.
3. NEXAFS measurements were carried out at the Surface, Interface and Nanostructure Science (SINS) beamline of the Singapore Synchrotron Light Source.

All of the PES and NEXAFS measurements were performed at room temperature (RT). The NEXAFS measurements were performed in total-electron yield (TEY) mode with a photon energy resolution of 0.1 eV. The linear polarization factor of synchrotron light at the SINS beamline was measured to be about 0.95.

Si substrates and freshly cleaved HOPG substrates were thoroughly degassed in the UHV chamber at around 730K overnight before deposition. F16CuPc and DIP were evaporated in situ from separate Knudsen cells.

## Experiments Results :1. morphology

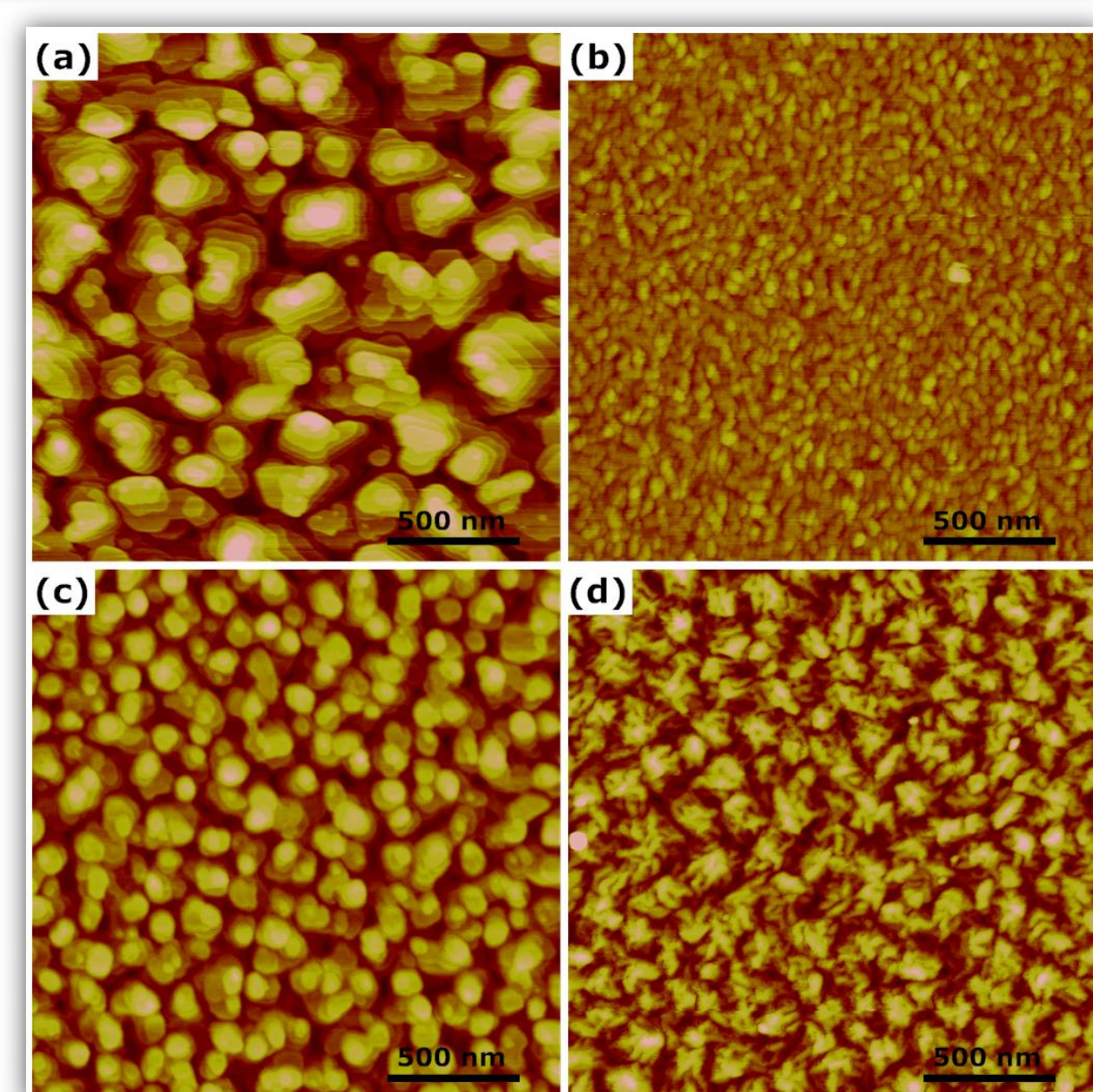


Fig 2. AFM morphology images (2x2um, 15nm scale range). (a) DIP on SiO<sub>2</sub>, (b) F16CuPc on SiO<sub>2</sub>, (c) DIP on F16CuPc on SiO<sub>2</sub>, (d) F16CuPc on DIP on SiO<sub>2</sub>

## 2. Lying-down heterojunction

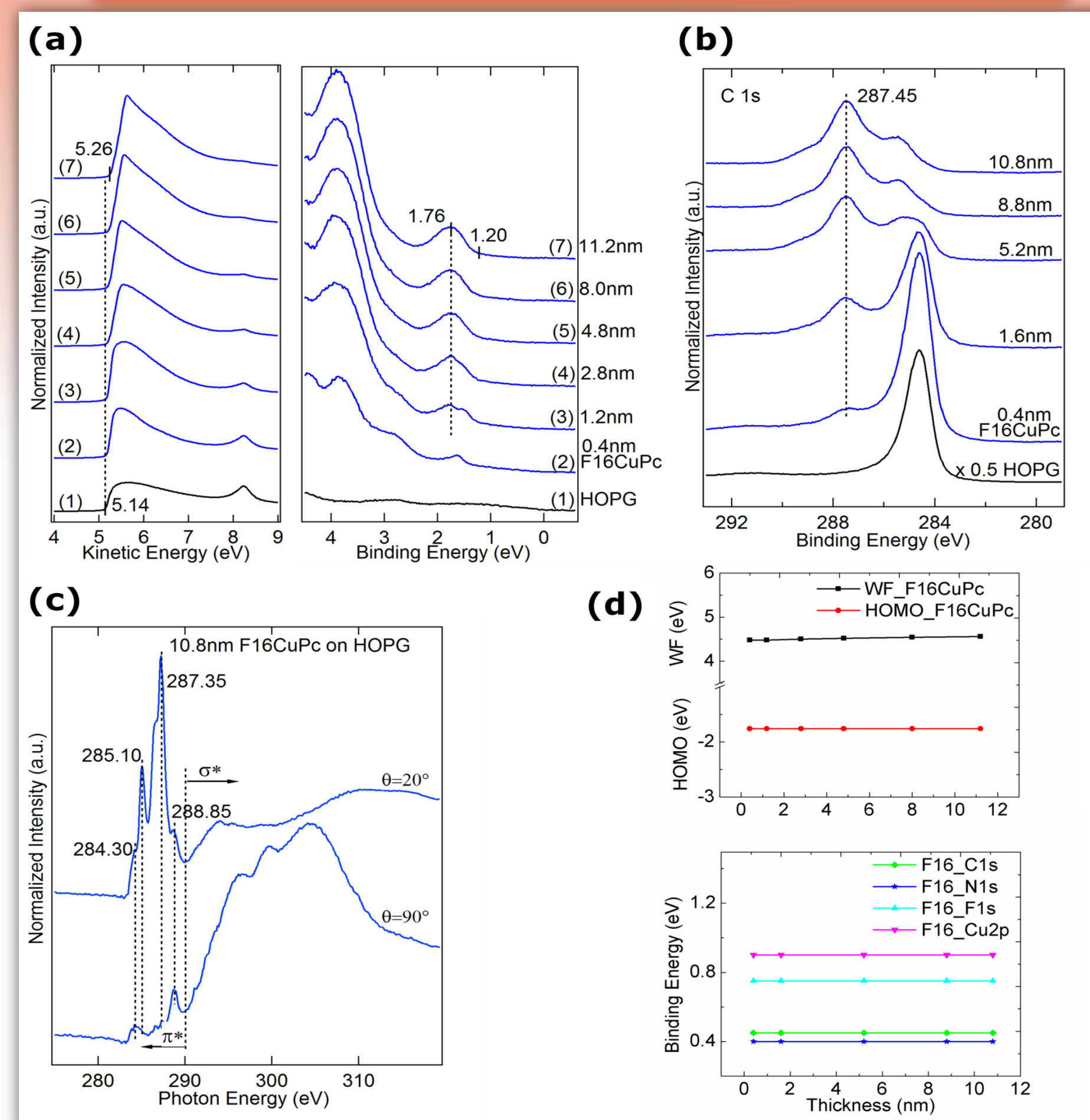


Fig 3. (a) UPS spectra at low kinetic energy region (left) and the low-binding energy region near the Fermi level (right) during the deposition of F16CuPc on HOPG. (b) XPS C1s core level evolution for F16CuPc on HOPG. (c) Angle-dependent C k-edge NEXAFS spectra for F16CuPc on HOPG. (d) HOMO peak position, work function (up) and core level (down) of lying F16CuPc on HOPG as a function of film thickness.

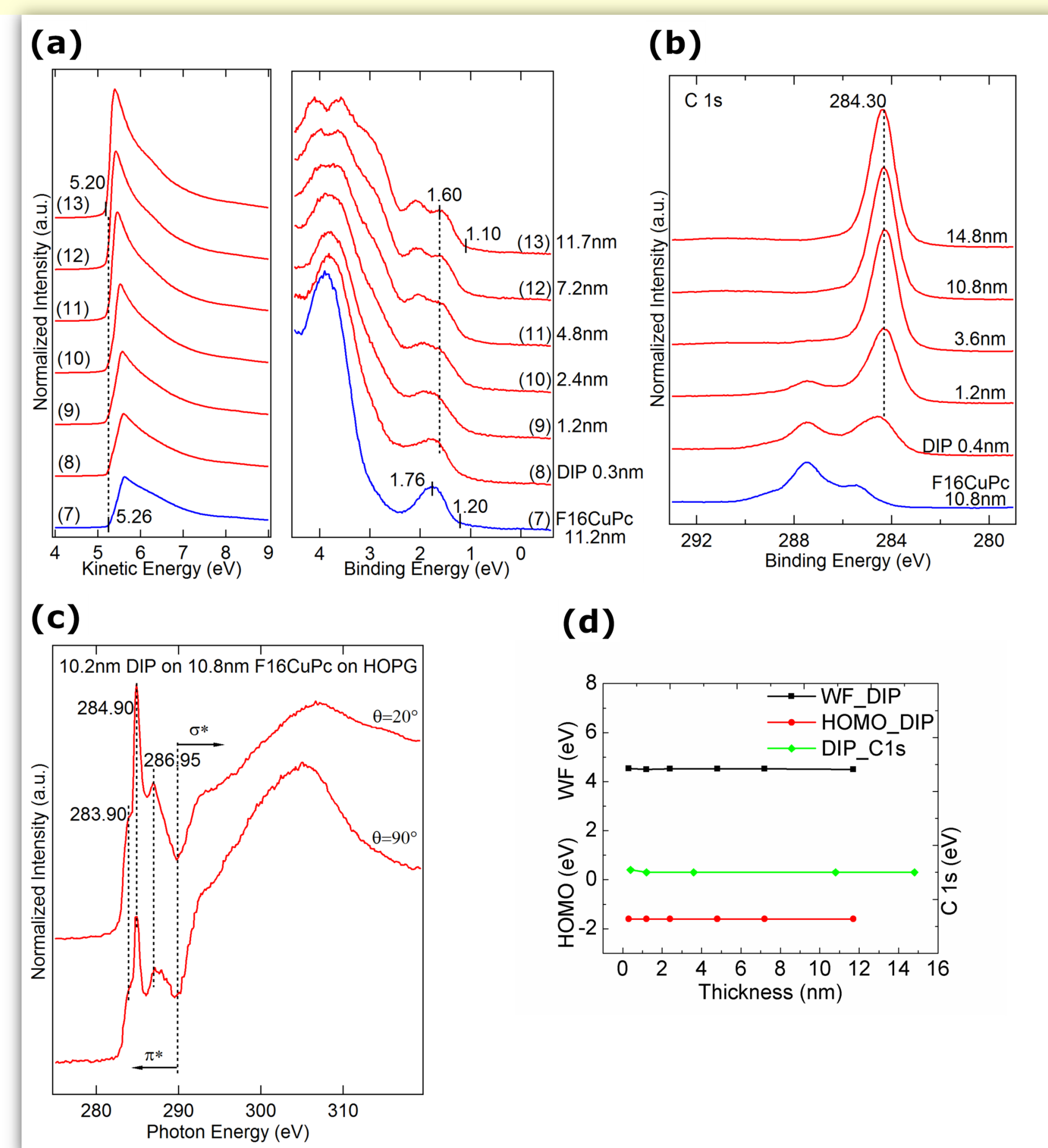


Fig 4. (a) UPS spectra at low kinetic energy region (left) and the low-binding energy region near the Fermi level (right) during the deposition of DIP on F16CuPc/HOPG. (b) XPS C1s core level evolution for DIP/F16CuPc heterojunction. (c) Angle-dependent C k-edge NEXAFS spectra for DIP on F16CuPc/HOPG. (d) HOMO peak position, work function and C1s core level of lying-down DIP on F16CuPc/HOPG as a function of film thickness.

## 3. Standing-up heterojunction

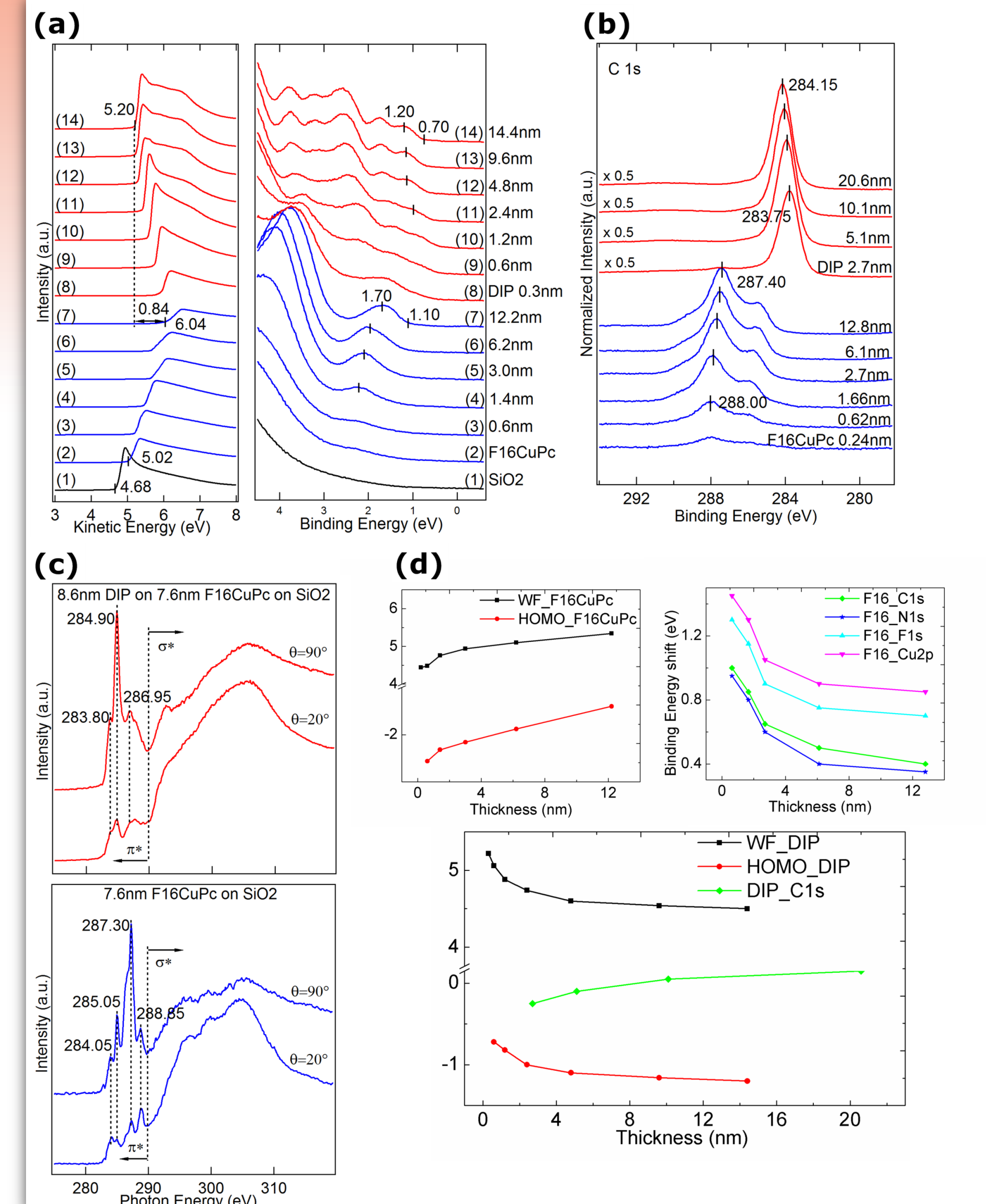


Fig 5. (a) UPS spectra at low kinetic energy region (left) and the low-binding energy region near the Fermi level (right) during the deposition of DIP on F16CuPc on SiO<sub>2</sub>. (b) XPS C1s core level evolution for DIP/F16CuPc heterojunction. (c) Angle-dependent C k-edge NEXAFS spectra for F16CuPc on SiO<sub>2</sub> (down) and DIP on F16CuPc/SiO<sub>2</sub> (up). (d) HOMO peak position, work function and core level of standing F16CuPc/SiO<sub>2</sub> (up) and standing DIP/F16CuPc/SiO<sub>2</sub> (down) as a function of film thickness.

## 4. Energy level diagrams

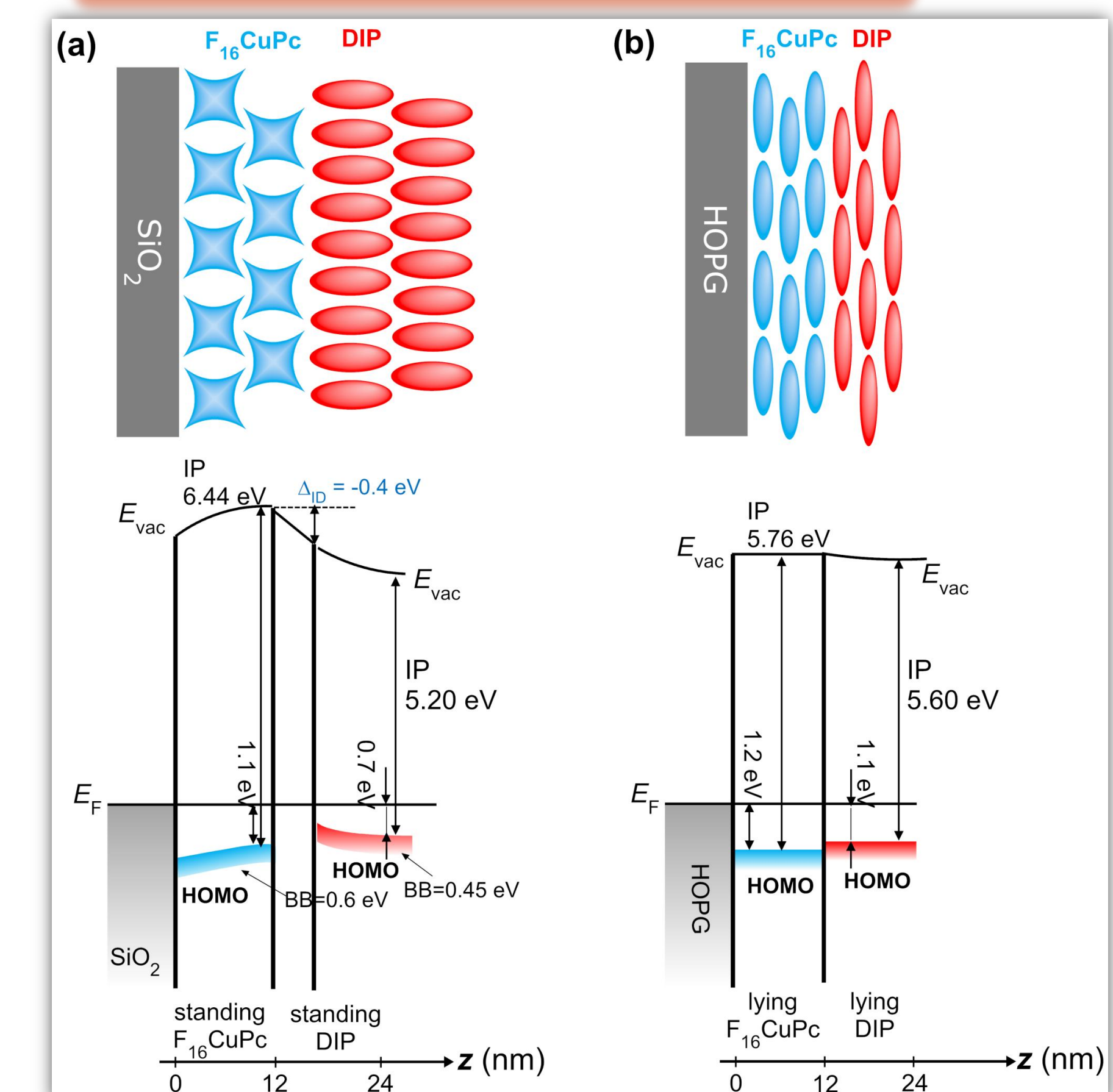


Fig 6. Summary of the molecular orientations and schematic energy level alignment diagrams for the F16CuPc/DIP heterojunctions on different substrates.

## Conclusions

- ❖1. F16CuPc adopt standing-up configuration on SiO<sub>2</sub> while lying-down on HOPG substrate, and DIP have the same molecular orientation of the underlying F16CuPc thin films as revealed by NEXAFS.
- ❖2. The ionization potential (IP) of the ordered organic thin films depends on the molecular orientation, the F16CuPc have higher IP for standing-up configuration while DIP have higher IP at lying-down orientation.
- ❖3. Observed orientation dependent interfacial charge transfer and energy level alignment at the DIP/F16CuPc heterojunctions. There is a band bending behavior and interfacial charge transfer in the standing-up configuration OOHs.

## References

- Chen, W., Qi, D.-C., Huang, H., Gao, X. and Wee, A. T. S. (2011), Adv. Funct. Mater., 21: 410–424.  
Braun, S., Salaneck, W. R. and Fahlman, M. (2009), Adv. Mater., 21: 1450–1472.