

Fluctuation in band structures of pentacene/Au(111) investigated by scanning tunneling spectroscopy

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SUMMARY:

We investigate local spatial fluctuation in the band structure of pentacene thin films, which is a typical material of organic field effect transistors, using scanning tunneling microscopy/ spectroscopy (STM/STS). We found a localized gap state in the band gap of pentacene, which locates at the defect (etch-pit) formed on SAM/Au(111). We propose that the gap state originates from the hybrid orbital between pentacene molecules and Au atoms around the etch-pit.

INTRODUCTION:

In organic semiconductor devices, material inhomogeneity of defect, impurity, and grain boundary results in spatial fluctuation in the band structures. It has been well established that spatial fluctuation dramatically impairs device performance of, for example, carrier mobility. However, no direct observation of such fluctuation is reported. Here we directly observe the spatial distribution in the band structure of the organic semiconductor using STM/STS.

EXPERIMENTALS:

A pentacene thin film was prepared by vacuum deposition at room temperature on an alkanethiol self-assembled monolayer (SAM) on a Au(111) substrate. Using STM, we confirmed that pentacene molecules are orderly packed with atomic steps. For STS measurement, I-V curves were measured at different areas, and the dI/dV -V curves were numerically calculated. To obtain the spatial distribution of the band structure, the values of dI/dV for different V s were imaged.

RESULTS AND DISCUSSION:

The dI/dV -V curves reflect that a new state (gap state) is formed in the band gap of pentacene. The spatial distribution of the gap state has no relation with surface topography. We found that the gap state locates at the defect, etch-pit formed on SAM/Au(111). We propose that the gap state originates from the hybrid orbital between pentacene molecules and Au atoms around the etch-pit.

CONCLUSIONS:

We visualized the spatial distribution of the gap state for pentacene/SAM/Au(111), and proposed the mechanism for the origin of the gap state.