Low-temperature STM/STS Studies on Local Density of States of Phthalocyanine Molecules on Metal Surfaces

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Adsorption of molecules on metal surfaces produces new electronic states induced by orbital interactions between the molecules and the surfaces. Scanning tunneling microscopy (STM) and spectroscopy (STS) enable us to observe local density of states (LDOS) based on dI/dV images recorded simultaneously with topographic images in real space. In this study, LDOS of cobalt phthalocyanine (CoPc) molecules on Cu(100) and Au(111) surfaces were observed by STM/STS at 5K in ultrahigh vacuum[1].

Figures 1(a) and 1(b) show dI/dV spectra of a CoPc molecule on Au(111) and Cu(100), respectively. The insets show STM images of CoPc. The dI/dV spectra were recorded at two different points on each molecule marked (1)-(4). In Fig. 1(a), there are four peaks at the bias voltages of -0.8V (H-1), -0.5V (H), -0.3V (D) and +1.1V (L). Comparing the results to those based on photoemission spectroscopy and molecular orbital (MO) calculation, peak H, H-1, L and D were assigned to the highest occupied MO (HOMO), the next HOMO, the lowest unoccupied MO (LUMO) and d-orbital of the center cobalt atom, respectively. While there was no additional peak between HOMO and LUMO in Fig. 1(a), new electronic states indicated as I_1 and I_2 appeared in Fig. 1(b). These states were thought to be generated by the hybridization between MOs of CoPc and electronic states of Cu(100) surfaces. The origin of the adsorption-induced states will be discussed based on the dI/dV images of the molecule and MO calculations.

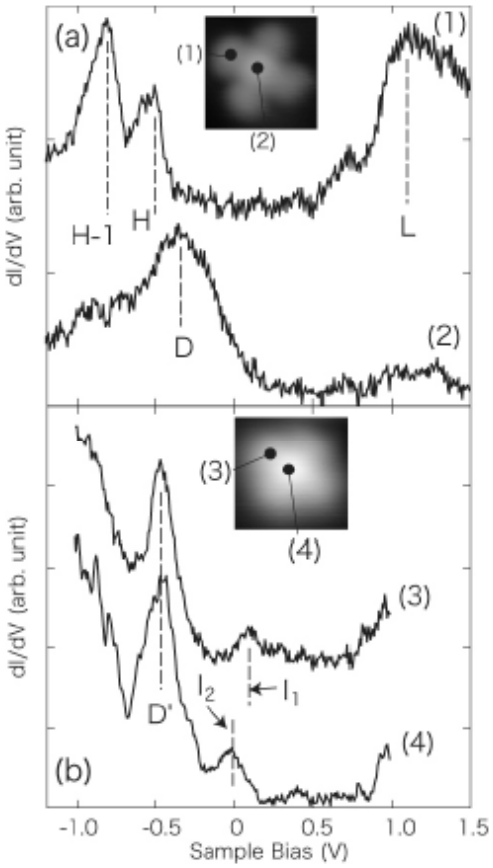

Figure 1. The dI/dV spectra of CoPc on Au(111) (a) and Cu(100) (b). The spectra were recorded at the position marked on the molecule in the insets.

[1] M. Takada and H. Tada, Ultramicroscopy **105**, 22-25 (2005); Jpn. J. Appl. Phys. **44**, 5332-5335 (2005); Mol. Cryst. Liq. Cryst. **455**, 93-97 (2006).