Spin-Polarized Electronic States of Mn-phthalocyanine Ultrathin Films by Ultraviolet Photoelectron Spectroscopy

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Transition metal-phthalocyanines (Pcs) are a versatile class of π-conjugated organic semiconductors and has been expected as promising optoelectronic/magnetic materials due to the tunable electron/spin function via 3d-electron derived molecular orbital (MO). However, systematic information on the electronic structure as well as the electron/spin configuration of such organometallic complexes is very limited. Moreover, effects of molecule-substrate and intermolecular interaction on the electronic structure are still not known for the molecular thin films. To characterize the electronic structure of the molecule itself and the molecule/metal interface, we have studied various monolayers of metal (Mn-, Fe-, Co-, Ni-, Cu-, Zn-) Pcs on graphite and Ag(111) by ultraviolet photoelectron spectroscopy (UPS) combined with multiple-scattering theory.

Figure 1 shows the HeI UPS of MnPc monolayer on graphite (HOPG) and Ag(111). The electronic states of MnPc/HOPG are nearly conserved as in the gaseous states due to a weak physisorption. From the emission angle and photon energy dependences, band A is ascribed to singly occupied $3d_{z^2}$-derived band (a_{1g}), while band B is to 2p(π)-derived band (a_{1u}) as seen in other Pc molecules [1]. On the other hand, the UPS features are changed drastically for the MnPc/Ag(111). The energy position and angular distribution of band B is similar to that of the MnPc/HOPG. Band A is, however, appeared at lower energy side and angular distribution is markedly different from a_{1g} MO. It indicates that spin configuration of MnPc is changed due to symmetry breaking with the molecule/substrate interaction [2]. A possible electron/spin configuration will be discussed by comparison with the theoretical calculations.

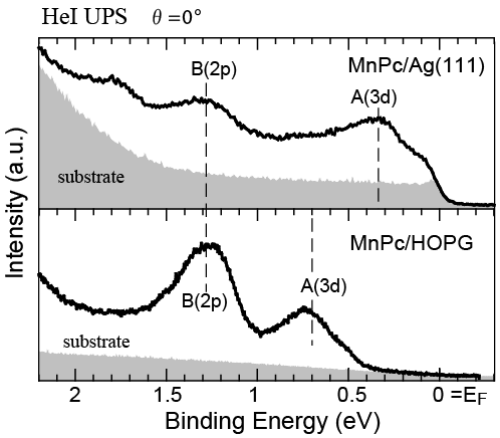

Figure 1 HeI UPS of MnPc monolayer deposited on the HOPG and Ag(111) substrate measured at 295 K.

[1] N. Ueno *et al*., Appl. Phys. A 92 (2008) 495.
[2] N. Marom, L. Kronik, Appl. Phys. A 95 (2009) 165.