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 \(\pi\)-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\textsubscript{z}\textsuperscript{2}-derived band \((a_{1g})\), while band B is to 2p(\(\pi\))-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.