UVSOR Facility

KOSUGI, Nobuhiro KATOH, Masahiro SHIGEMASA, Eiji TANAKA, Kiyohisa IWAYAMA, Hiroshi MATSUNAMI, Masaharu OHIGASHI, Takuji KONOMI, Taro HORIGOME, Toshio HASUMOTO, Masami YAMAZAKI, Jun-ichiro HAYASHI, Kenji KONDO, Naonori SAKAI, Masahiro **TESHIMA**, Fumitsuna TOKUSHI, Tetsunari INAGAKI, Yuichi HAYASHI, Ken-ichi MINAKUĆHI, Aki HAGIWARA, Hisayo

Director Professor Associate Professor Associate Professor Assistant Professor Assistant Professor Assistant Professor Assistant Professor Technical Associate Technical Associate Technical Associate **Technical Associate** Technical Associate Technical Associate Technical Associate **Technical Fellow** Technical Fellow **Technical Fellow Technical Fellow** Secretary



Outline of UVSOR

Since the first light in 1983, UVSOR has been successfully operated as one of the major synchrotron light sources in Japan. After the major upgrade of the accelerators in 2003, UVSOR was renamed to UVSOR-II and became one of the world brightest low energy synchrotron light source. In 2012, it was upgraded again and has been renamed to UVSOR-III. The brightness of the electron beam was increased further. Totally, six undulators were installed. The storage ring is operated fully in the top-up mode, in which the electron beam intensity is kept constant.

The UVSOR accelerator complex consists of a 15 MeV injector linac, a 750 MeV booster synchrotron, and a 750 MeV storage ring. The magnet lattice of the storage ring consists of four extended double-bend cells with distributed dispersion function. The storage ring is normally operated under multibunch mode with partial filling. The single bunch operation is also conducted about two weeks per year, which provides pulsed synchrotron radiation (SR) for time-resolved experiments.

Eight bending magnets and six undulators are available for providing SR. The bending magnet with its radius of 2.2 m provides SR with the critical energy of 425 eV. There are fifteen beam-lines operational. They can be classified into two categories. Eleven of them are the so-called "Open beamlines," which are open to scientists of universities and research institutes belonging to the government, public organizations, private enterprises and those of foreign countries. The other three beam-lines are the so-called "In-house beamlines," which are mainly used by the research groups within IMS. We have 1 soft X-rays (SX) station equipped with a double-crystal monochromator, 7 EUV and SX stations with a grazing incidence monochromator, 2 (far) infrared station equipped with FT interferometers and 1 beam-line for light source development without monochromator.



Figure 1. UVSOR electron storage ring and synchrotron radiation beam-lines.

Collaborations at UVSOR

Variety of investigations related to molecular/material science is carried out at UVSOR by IMS researchers. In addition, many researchers outside IMS visit UVSOR to conduct their own research works. The number of visiting researchers per year tops about 800, whose affiliations extend to 60 different institutes. International collaboration is also pursued actively and the number of visiting foreign researchers reaches over 80, across about 10 countries. UVSOR invites new/continuing proposals for research conducted at the open beamlines twice a year. The proposals from academic and public research organizations (charge-free) and from enterprises (charged) are acceptable. The fruits of the research activities using SR at UVSOR are published as a UVSOR ACTIVITY REPORT annually.

Recent Developments

In spring, 2013, we had two month shut-down for a reconstruction work at an undulator beam-line BL5U. The undulator at BL5U, which had been constructed about 20 years ago, was remodeled. Now it has become capable of producing any polarization, such as horizontal and vertical linear polarizations and left and right circular polarizations.

The endstation of BL5U has started to be renewed to perform higher energy resolution ARPES experiments. This endstation will have new capability to obtain spin- and spatialdependence of the electronic structure of solids using new spin detector and micro-focused beam. This beam-line will be open for users from 2015.



Figure 2. Current situation of new ARPES beam-line BL5U.

Reserch Highlight

Solid-state functionalities of organic molecules are governed not only by individual molecular properties but also by their intermolecular interactions. This concerted interplay dominates a key process of the electric conduction in functional molecular systems. In this work, we have investigated the intermolecular energy-*vs*-momentum $E(\mathbf{k})$ relation, originating from the molecular stacking periodicity, of sub-100meV scale in metal phthalocyanine (MPc) crystalline films. The small $E(\mathbf{k})$ relation of MPc with different terminal groups and central metals are sensitive and essential to characterize the intermolecular interaction in terms of the intermolecular distance, the molecular conformation, and the orbital symmetry.

Figure 3 shows the emission angle (θ) dependence of the angle-resolved photoemission (ARPES) spectra and its intensity map for the flat-lying monolayer and crystalline films of ZnPc on Au(111) at 15 K. For the monolayer, the dispersive and non-dispersive peaks appear around the binding energy (E_b) of 0 ~ 0.32 eV and 0.74 eV, respectively. The parabolic dispersion at $E_b = 0 \sim 0.32$ eV is derived from the Shockley State (SS) of the Au(111) surface, which is modified by the complex interplay of molecule–substrate interactions. The non-dispersive peak at $E_b = 0.74$ eV is derived from the highest occupied molecular orbital (HOMO) of C 2p (π) character in ZnPc. The observed HOMO-peak intensity shows

a sharp θ dependence with the maximum at $\theta = 34^{\circ}$. This is due to the reflection of the spatial electron distribution of HOMO. For the ZnPc crystalline film, the SS band of Au(111) is suppressed and the HOMO peak is stabilized as $E_b \sim 1.3$ eV. Since the ZnPc molecule deposited on Au(111) shows the Stranski-Krastanov growth, the quite weak substrate signal of $E_{\rm F}$ appears and is utilized for the energy calibration for the precise E(k) measurement. The θ dependence of the HOMOpeak intensity in the ZnPc crystalline film is almost the same as that in the ZnPc monolayer; that is, the molecular orientation indicates the layer-by-layer growth in the crystalline domain and induces orbital delocalization. Indeed, the HOMO peak of the ZnPc crystalline film shows a small dispersive behavior with θ . Such a dispersive behavior is not observed in the monolayer film and is related to the delocalized band formation.

In order to investigate the k component along the π - π stacking direction (k_{\perp}), we measured the normal emission ARPES as a function of the photon energy (hv) for crystalline films of various MPc (H₂Pc, MnPc, CoPc, ZnPc, and F₁₆ZnPc) on Au(111) at 15 K. From this systematic experiment, we revealed quite small but different $E(k_{\perp})$ relations. The transfer integral (t_{\perp}) of the C 2p band is found to be dependent on the intermolecular distance (a_{\perp}) with the 75±5 meV/Å relation. Furthermore, we observed the different dispersion phase and periodicity, depending on the terminal group and central metal in MPc, which originate from the site-specific intermolecular interaction induced by substituents.¹



Figure 3. The θ dependence of the ARPES spectra (hv = 45 eV) and its intensity map for the monolayer and crystalline films of ZnPc on Au(111) at 15 K.

Reference

1) H. Yamane and N. Kosugi, Phys. Rev. Lett. 111, 086602 (2013).