RESEARCH FACILITIES

The Institute includes five research facilities. This section describes their latest equipment and activities. For further information please refer to previous IMS Annual Review issues (1978–2013).

UVSOR Facility

KOSUGI, Nobuhiro	Director
KATOH, Masahiro	Professor
SHIGEMASA, Eiji	Associate Professor
TANAKA, Kiyohisa	Associate Professor
IWAYAMA, Hiroshi	Assistant Professor
MATSUNAMI, Masaharu	Assistant Professor
OHIGASHI, Takuji	Assistant Professor
KONOMI, Taro	Assistant Professor
HORIGOME, Toshio	Technical Associate
HASUMOTO, Masami	Technical Associate
YAMAZAKI, Jun-ichiro	Technical Associate
HAYASHI, Kenji	Technical Associate
KONDO, Naonori	Technical Associate
SAKAI, Masahiro	Technical Associate
TESHIMA, Fumitsuna	Technical Associate
TOKUSHI, Tetsunari	Technical Fellow
INAGAKI, Yuichi	Technical Fellow
HAYASHI, Ken-ichi	Technical Fellow
MINAKUCHI, Aki	Technical Fellow
HAGIWARA, Hisayo	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 multi-bunch 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 beam-lines," 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, 3 VUV stations with a normal 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 spatial-dependence 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 $E(\boldsymbol{k})$ relation, originating from the molecular stacking periodicity, of sub-100-meV scale in metal phthalocyanine (MPc) crystalline films. The small $E(\boldsymbol{k})$ 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 ~ 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 θ = 34°. 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 ~ 1.3 eV. Since the ZnPc molecule deposited on Au(111) shows the Stranski-Krastanov growth, the quite weak substrate signal of E_F appears and is utilized for the energy calibration for the precise $E(\boldsymbol{k})$ measurement. The θ dependence of the HOMO-peak 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 $\boldsymbol{k}$ component along the π-π stacking direction ($\boldsymbol{k}_\perp$), we measured the normal emission ARPES as a function of the photon energy ($h\nu$) for crystalline films of various MPc (H_2Pc, MnPc, CoPc, ZnPc, and F_{16}ZnPc) on Au(111) at 15 K. From this systematic experiment, we revealed quite small but different $E(\boldsymbol{k}_\perp)$ 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)]

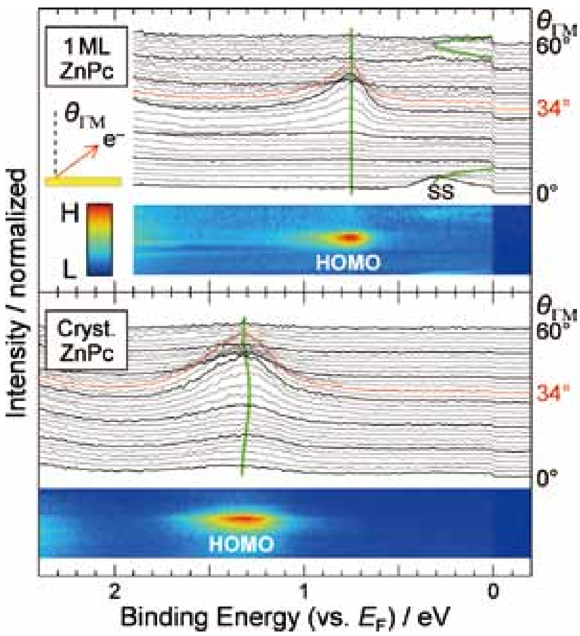

Figure 3. The θ dependence of the ARPES spectra ($h\nu$ = 45 eV) and its intensity map for the monolayer and crystalline films of ZnPc on Au(111) at 15 K.

Reference

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

Laser Research Center for Molecular Science

OKAMOTO, Hiromi	Director, Professor
KATOH, Masahiro	Professor
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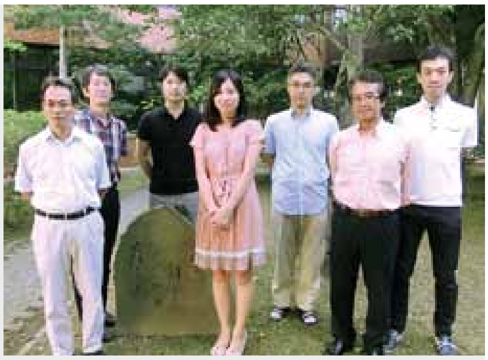
TAIRA, Takunori	Associate Professor
FUJI, Takao	Associate Professor
ISHIZUKI, Hideki	Assistant Professor
NOMURA, Yutaka	Assistant Professor
OKANO, Yasuaki	Technical Associate
MASUDA, Michiko	Secretary
KAWAI, Shigeko	Secretary



The Center aims to develop new experimental apparatus and methods to open groundbreaking research fields in molecular science, in collaboration with the Department of Photo-Molecular Science. Those new apparatus and methods will be served as key resources in advanced collaborations with the researchers from the community of molecular science. The main targets are (1) advanced photon sources covering wide energy ranges from terahertz to soft X-day regions; (2) novel quantum-control schemes based on intense and ultrafast lasers; and (3) high-resolution optical imaging and nanometric microscopy. The center also serves as the core of the joint research project "Extreme Photonics" between IMS and RIKEN.

Two of full-time associate professors and their research groups belong to the Center. The groups promote research projects targeting mainly on developments of novel laser light sources for molecular science. The Center also possesses several general-purpose instruments for laser-related measurements, and lends them to researchers in IMS who conduct laser-based studies, so as to support and contribute to their advanced researches.

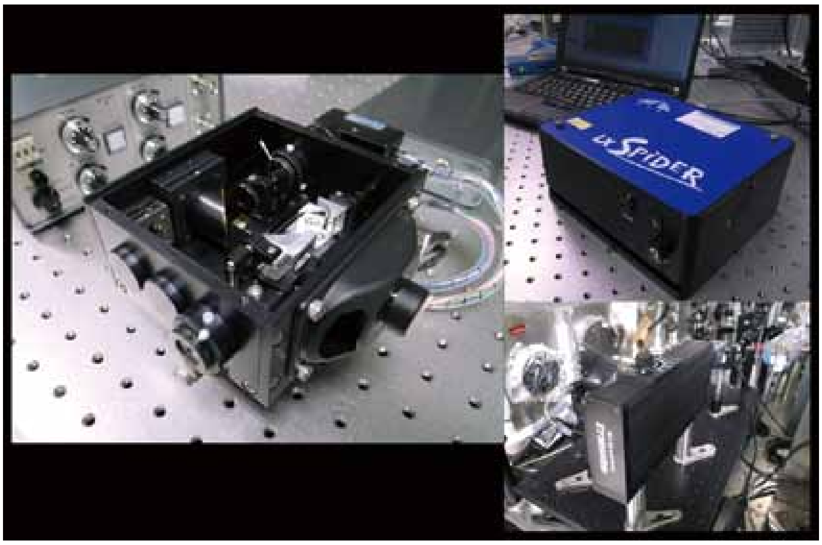


Figure 1. (left) A Fringe-Resolved Autocorrelation (FRAC) apparatus for sub-10 fs pulse characterization designed in the Center. (upper right) Spectral Phase Interferometry for Direct Electric-Field Reconstruction (SPIDER) and (lower right) Frequency-Resolved Optical Gating (FROG) apparatuses for general-purpose ultrashort pulse characterization.

Instrument Center

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MIZUKAWA, Tetsunori	Technical Associate
MAKITA, Seiji	Technical Associate
NAKANO, Michiko	Technical Associate
UEDA, Tadashi	Technical Associate
OTA, Akiyo	Secretary
NAKAGAWA, Nobuyo	Secretary

Instrument Center was organized in April of 2007 by integrating the general-purpose facilities of Research Center for Molecular Scale Nanoscience and Laser Research Center for Molecular Science. The mission of Instrument Center is to support the in-house and external researchers in the field of molecular science, who intend to conduct their research by utilizing general-purpose instruments. The staffs of Instrument Center maintain the best condition of the machines, and provide consultation for how to use them. The main instruments the Center now maintains in Yamate campus are: Nuclear magnetic resonance (NMR) spectrometers (JEOL JNM-ECA 920, JNM-ECA 600, and JNM-LA500, JNM-ECS400, and Bruker AVANCE800), matrix assisted laser desorption ionization (MALDI) mass spectrometer (Voyager DE-STR), powder X-ray diffractometer (Rigaku RINT-Ultima III), circular dichroism (CD) spectrometer (JASCO JW-720WI), differential scanning calorimeter (MicroCal VP-DSC), and isothermal titration calorimeter (MicroCal iTC200), scanning electron microscope (SEM; JEOL JEM-6700F(1), JED-2201F), focused ion beam (FIB) machine (JEOL JEM-9310FIB(P)), elemental analyzer (J-Science Lab Micro Corder JM10). In the Myodaiji campus, the following instruments are installed: Electron spin resonance (ESR) spectrometers (Bruker E680, E500, EMX Plus), NMR spectrometer (Bruker AVANCE600), superconducting quantum interference devices (SQUID; Quantum Design MPMS-7 and MPMS-XL7), powder X-ray diffractometer (MAC Science MXP3), solution X-ray diffractometer (Rigaku NANO-Viewer), single-crystal X-ray diffractometers (Rigaku Mercury CCD-1, CCD-2, RAXIS IV, and 4176F07), thermal analysis instruments (TA TGA2950, DSC2920, and SDT2960), fluorescence spectro-photometer (SPEX Fluorolog2), X-ray fluorescence spectrometer (JEOL JSX-3400RII), UV-VIS-NIR spectro-photometer (Hitachi U-3500), Raman microscope (Renishaw INVIA REFLEX532), excimer/dye laser system (Lambda Physics LPX105i/LPD3002), Nd^+: YAG-laser pumped OPO laser (Spectra Physics GCR-250/Lambda Physics Scanmate OPPO), excimer laser (Lambda Physics Complex 110F), and picosecond tunable laser system (Spectra Physics Tsunami/Quantronix Titan/Light Conversion TOPAS), SEM (Hitachi SU6600), electron spectrometers for chemical analysis (ESCA) (Omicron EA-125), high-resolution transmission electron microscope (TEM; JEOL JEM-3100FEF), and FTIR spectrometer (Bruker IFS 66v/S). In the fiscal year of 2013, Instrument Center accepted almost 140 applications from institutions outside IMS. Instrument Center also maintains helium liquefiers in the both campus and provides liquid helium to users. Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute. The staffs of Instrument Center provide consultation for how to treat liquid helium, and provide various parts necessary for low-temperature experiments. Instrument Center supports also the Inter-University Network for Common Utilization of Research Equipments.

Figure 1. 600 MHz NMR spectrometer (JEOL JNM-ESA600).

Figure 2. Pulse ESR for Q-band (Bruker E680).

Figure 3. Raman microscope (Renishaw INVIA REFLEX532).

Equipment Development Center

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KONDOU, Takuhiko	Technical Associate
YOSHIDA, Hisashi	Technical Associate
UTCHIYAMA, Kouichi	Technical Associate
TOYODA, Tomonori	Technical Associate
TAKADA, Noriko	Technical Associate
NAKANO, Michiko	Technical Associate
SUGITO,Shouji	Technical Fellow
URANO, Hiroko	Secretary

Researches and developments of novel instruments demanded in the forefront of molecular science, including their design and fabrication, are the missions of this center. Technical staffs in the two work sections, mechanics and electronics, are engaged in developing state-of-the-art experimental instruments in collaboration with scientists. We expanded our service to other universities and research institutes since 2005, to contribute to the molecular science community and to improve the technology level of the center staffs. A few selected examples of our recent developments are described below.

ARM-Microcontroller-Based Rotary Solenoid Driver

WA laser-shutter device, which can block a laser beam synchronizing with external control signals as trigger, is one of the basic elements in optical systems. In this work, we have developed a driver unit to control a shutter device, which consists of a bi-stable rotary-solenoid and a shutter plate, operated with TTL level trigger at a repetition rate up to 10 Hz (Figure 1).

Specifications of the driver are as follows: First, it detects the rising edge of the trigger, then, generates a Phase-A output to drive the rotary solenoid clockwise with a predetermined duration. Next, it detects the falling edge of the trigger, and generates a Phase-B output to drive the solenoid counterclockwise with a predetermined duration. The tunable ranges of Phase-A and -B durations are from 1 ms to 99 ms with the step of 1 ms.

Conventionally, we used a combination of standard logic ICs for driving a circuit synchronized with a trigger. In this case, we adopted the module of LPC1114FBD48/302, the ARM microcontroller by NXP. We set one of the pins of ARM module as an input, and set interrupts on both edges of the trigger (rising and falling). ARM module identifies rising or falling edge in the interrupt handler, and outputs Phase A or Phase B. (Figure 2).

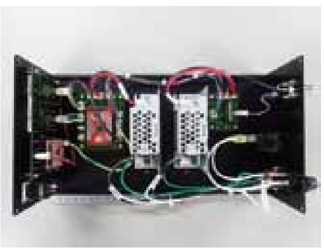

Figure 1. Photo of the rotary solenoid driver.

The duration of the each output is adjustable with a rotary encoder which is connected to the ARM module. Increasing or decreasing of the value is performed by detecting the rotation direction of the rotary encoder. The value is displayed on a LCD by another ARM module. We adopted I2C for communication between two ARM modules.

Figure 2. The input–output characteristics of the rotary solenoid driver.

Cathode Plug for Superconducting Electron Emitter

A new electron source is required for the development of next generation synchrotron radiation system. A cathode plug that will be used for photo-cathode with back-side irradiation has been fabricated (Figure 3). The plug is designed to be able to hold a photo-cathode substrate on the top, and can be fixed with screw on the cathode holder. The photo-cathode substrate, whose size is 5 × 5 × 0.5 mm^3, is requested to stay in the same plane with the plug's top-edge plane, and therefore cannot be fixed by using a holding plate mounting on it. At the same time, fixing of the substrate by side-holding makes it bending and inclining, which arises another undesirable problems. In order to address these issues, we have designed a new substrate-holding cathode plug with elastic parallel hinge structure. The tightness of the hinge was optimized to meet the best result of finite-element-method calculation by ANSYS program (Figure 4), so that accurate fixing of photo-cathode substrate has finally been achieved.

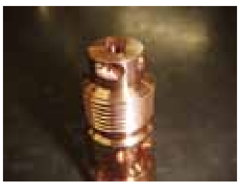

Figure 3. Cathode plug for electron emission.

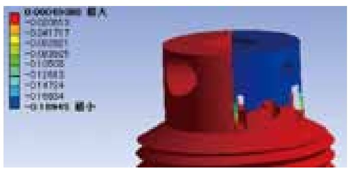

Figure 4. Analysis result for the elastic hinge calculated by ANSYS.

Research Center for Computational Science

SAITO, Shinji	Director, Professor
EHARA, Masahiro	Professor
OKUMURA, Hisashi	Associate Professor
OONO, Hitoshi	Assistant Professor
ISHIDA, Tateki	Assistant Professor
FUKUDA, Ryoichi	Assistant Professor
ITOH, G. Satoru	Assistant Professor
MIZUTANI, Fumiyasu	Technical Associate
NAITO, Shigeki	Technical Associate
SAWA, Masataka	Technical Associate
IWAHASHI, Kensuke	Technical Associate
MATSUO, Jun-ichi	Technical Associate
NAGAYA, Takakazu	Technical Associate
TOYA, Akiko	Secretary
ISHIHARA, Mayumi	Secretary

Research Center for Computational Science provides state-of-the-art computational resources to academic researchers in molecular science and related fields, *e.g.* quantum chemistry, molecular simulations, and solid state physics. The computer systems consist of Fujitsu PRIMERGY RX300, PRIME HPC FX10 and PRIMERGY CX250, SGI UV2000. 713 users in 185 project groups from a wide range of molecular science have used in 2013. Large scale calculations, for example the formation of fullerenes, conformation searches using non-Boltzmann ensemble methods, and nonlinear spectroscopy of liquids, have been performed with the systems. The Center also provides a number of application programs, for example Gaussian 09, GAMESS, Molpro, AMBER, and NAMD. The Center offers the Quantum Chemistry Literature Database, which has been developed by the Quantum Chemistry Database Group in collaboration with staff members of the Center. The latest release, QCLDB II Release 2013, contains 130,782 data of quantum chemical studies. Detailed information on the hardware and software is available on the web site (http://ccportal.ims.ac.jp/).

In addition to the provision of computational resources, the Center contributes to the so-called next-generation supercomputer project which is conducted by the government. In 2010, Computational Material Science Initiative (CMSI) was established, after the research field which consists of molecular science, solid state physics, and material science was selected as one of the research fields which scientific breakthroughs are expected by using the next-generation supercomputer. The Center contributes to CMSI by providing up to 20% of its computational resource.

Figure 1. Fujitsu PRIMERGY CX300.

Figure 2. SGI UV2000.

Okazaki Institute for Integrative Bioscience

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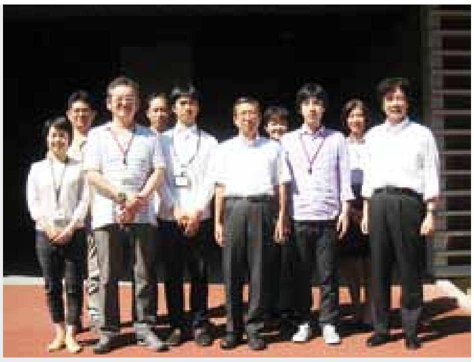
KATO, Koichi	Professor
IINO, Ryota	Professor
FUJII, Hiroshi	Associate Professor
KURIHARA, Kensuke	Research Associate Professor
KURAHASHI, Takuya	Assistant Professor
YOSHIOKA, Shiro	Assistant Professor
YAMAGUCHI, Takumi	Assistant Professor
MURAKI, Norifumi	IMS Research Assistant Professor
YAGI-UTSUMI, Maho	OIIB Research Assistant Professor
TANIZAWA, Misako	Secretary
TANAKA, Kei	Secretary



The main purpose of Okazaki Institute for Integrative Bioscience (OIIB) is to conduct interdisciplinary, molecular research on various biological phenomena such as signal transduction, differentiation and environmental response. OIIB, founded in April 2000, introduces cutting edge methodology from the physical and chemical disciplines to foster new trends in bioscience research. OIIB is a center shared by and benefited from all three institutes in Okazaki, thus encouraging innovative researches adequately in advance of academic and social demands. OIIB has started the research programs, "Okazaki ORION Project" and "BioNEXT Program" from 2014. The research groups of three full professors and one associate professor who have the position in IMS join OIIB to be involved in these research projects. The research activities of these groups are as follows.

Aono group is studying the bioinorganic chemistry of metalloproteins that show a novel function. They elucidated the structure and function relationships of the heme-based sensor proteins in which a heme was the active site for sensing gas molecules such as CO and O_2. They are also studying the structure and function relationships of transcriptional regulators and metal transport proteins that are responsible for metal homeostasis in bacteria. Iino group is studying operation mechanism of molecular machines using single-molecule techniques based on optical microscopy. Especially they focus on new rotary and linear molecular motors. In this year, they directly visualized rotation of a rotary molecular motor *Enterococcus hirae* V1-ATPase, and determined kinetic parameters for all elementary reaction steps of a linear molecular motor *Trichoderma reesei* Cel7A. They also applied single-molecule techniques to a synthetic molecular rotor double-decker porphyrin, and directly visualized the rotary motion for the first time. Kato group is studying structure, dynamics, and interactions of biological macromolecules using nuclear magnetic resonance (NMR) spectroscopy, X-ray crystallography, and other biophysical methods. In particular, they conducted studies aimed at elucidating the dynamic structures of glycoconjugates and proteins for integrative understanding of the mechanisms underlying their biological functions. In this year, they successfully elucidated the working mechanisms of proteasome assembly chaperones, Nas2 and Pba3–Pba4, the carbohydrate recognition modes of the cargo receptor complex, ERGIC-53–MCFD2, and the functional role of a product of a recently identified causative gene for dystroglycanopathy, AGO61. Fujii group is studying molecular mechanisms of metalloenzymes, which are a class of biologically important macromolecules having various functions such as oxygen transport, electron transfer, oxygenation, and signal transduction, with synthetic model complexes for the active site of the metalloenzymes. In this year, they studied molecular mechanisms of metalloenzymes relating to monooxygenation reactions and denitification processes. Kurihara group is studying an artificial cell based on a giant vesicle constructed from organic chemical approach. Their goal is to realize an artificial cell in which elements such as information, container and metabolism interact each other. In this year, they studied cross-catalytic vesicular system: A vesicle is reproduced by the catalyst which was synthesized in the vesicle, *i.e.* interaction between container and metabolism.

Safety Office

UOZUMI, Yasuhiro	Director
TOMURA, Masaaki	Assistant Professor
TANAKA, Shoji	Assistant Professor
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NAGATA, Masaaki	Technical Associate
UEDA, Tadashi	Technical Associate
TAKAYAMA, Takashi	Technical Associate
SAKAI, Masahiro	Technical Associate
MAKITA, Seiji	Technical Associate
KONDO, Naonori	Technical Associate
ONITAKE, Naoko	Secretary
TSURUTA, Yumiko	Secretary

The Safety Office was established in April 2004. The mission of the Office is to play a principal role in the institute to secure the safety and health of the staffs by achieving a comfortable workplace environment, and improvement of the working conditions. In concrete terms, it carries out planning, work instructions, fact-findings, and other services for safety and health in the institute. The Office is comprised of the following staffs: The Director of the Office, Safety-and-Health Administrators, Safety Office Personnel, Operational Chiefs and other staff members appointed by the Director General.

The Safety-and-Health Administrators patrol the laboratories in the institute once every week, and check whether the laboratory condition is kept sufficiently safe and comfortable to conduct researches. The Office also edits the safety manuals and gives safety training courses, for Japanese and foreign researchers.

A management system for chemical substances (mainly for commercial chemicals) was launched in May 2014 and has been steered by the Office. This office acknowledged a task force chaired by Prof. Yamamoto, which has drawn the specifications of the system up.