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 (1978–2012).

UVSOR Facility

KATOH, Masahiro	Director, Professor
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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
SAKAI, Masahiro	Technical Associate
HAYASHI, Kenji	Technical Associate
KONDO, Naonori	Technical Associate
TESHIMA, Fumitsuna	Technical Associate
TOKUSHI, Tetsunari	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. Twelve 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 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 of the Facility

In spring, 2012, we had three month shut-down for a reconstruction work towards UVSOR-III. The storage ring was successfully commissioned in July 2013. Although the operation was less stable for a few months than before, as the result of the fine tunings of the accelerators and of the vacuum conditioning via irradiation of synchrotron radiation, it has been improved gradually.

A scanning transmission X-ray microscope (STXM) beam-line, which was constructed as a part of the UVSOR-III upgrade program, was successfully commissioned.

Another upgrade program has been funded in 2012, in which the BL5U photoemission spectroscopy beam-line would be reconstructed as well as its light source, the variable polarization undulator. The designs were completed and the fabrications were started. The apparatuses will be installed in March 2014.

Figure 2. New STXM beam-line.

Reserch Highlight 2012

Topological insulators have become one of the model systems to study Dirac physics in solids. An essential ingredient in realizing a topological insulator is the parity inversion induced by the strong spin–orbit coupling. From this viewpoint, bismuth (Bi), which is virtually the heaviest non-radioactive element, has been the main building block. Nowadays many Bi alloys are known as topological insulators, although Bi itself is trivial. In these alloys, inhomogeneity may be introduced due to the complicated elemental composition. Therefore, searching for other ways to produce novel topological materials with a simple, well-defined structure, is important.

In this study, we have attempted to change the topological property of Bi by changing its lattice constant. We have fabricated Bi films on Bi_2Te_3 substrates and measured the band dispersion with angle-resolved photoemission spectroscopy. Due to the small in-plane lattice mismatch between Bi and Bi_2Te_3 (~3.6%), Bi can be grown epitaxially on Bi_2Te_3 from 1 BL.[1)] Figure 1(a) shows the band dispersion of a 7 BL Bi film on Bi_2Te_3. Compared to the 7 BL Bi film grown on Si(111)-7×7 [Figure 1(b)], the band dispersion is significantly different near the Γ point. This band dispersion was reproduced by ab inito calculations for a free standing Bi slab when the experimentally obtained lattice parameters were used. Furthermore, by calculating the 3D Z_2 topological for this strained Bi, we have found that the originally trivial Bi becomes nontrivial. Thus it is shown that the topological propertiy of Bi can be changed by inducing a small change in the lattice parameter.[2)]

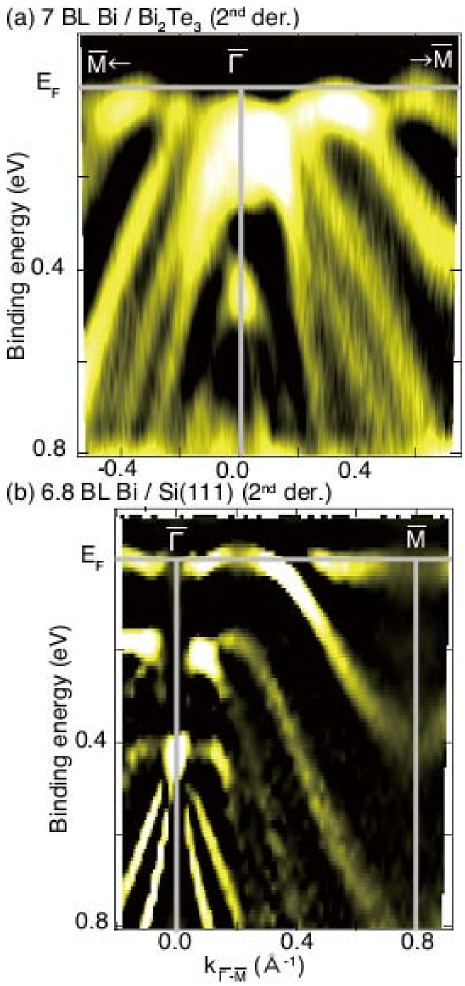

Figure 3. The band disperion of a 7 BL Bi(111) film grown on Bi_2Te_3 (a), and that on Si(111) (b).

References

1) T. Hirahara *et al.*, *Phys. Rev. Lett.* **107**, 166801 (2011).
2) T. Hirahara *et al.*, *Phys. Rev. Lett.* **109**, 227401 (2012).

Laser Research Center for Molecular Science

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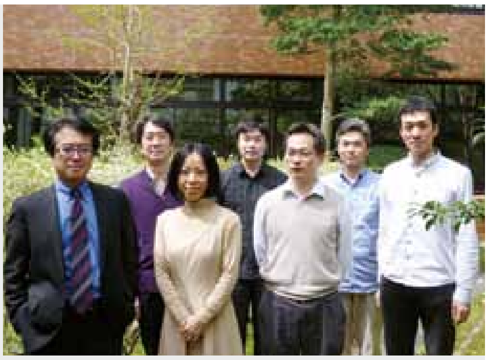
FUJI, Takao	Associate Professor
ISHIZUKI, Hideki	Assistant Professor
NOMURA, Yutaka	Assistant Professor
OKANO, Yasuaki	Technical Associate
KAWAI, Shigeko	Secretary
MASUDA, Michiko	Secretary



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.

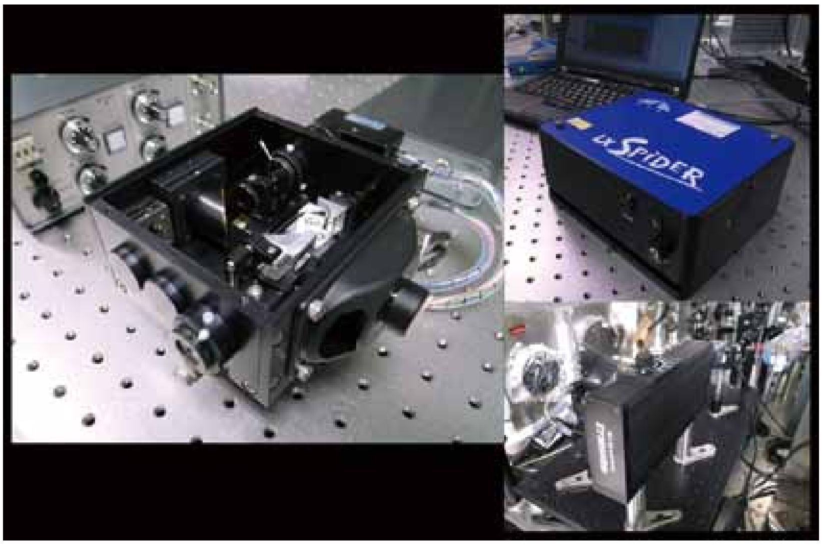


Figure 1. (left) A Fringe-Resolved Autocorrelation (FRAC) apparatus for sub-10 fs pulse characterization designed in the Center. (upper right) Spectral Phase Interferometry for Direct Electric-Field Reconstruction (SPIDER) and (lower right) Frequency-Resolved Optical Gating (FROG) apparatuses for general-purpose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

Instrument Center

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MIZUKAWA, Tetsunori	Technical Associate
MAKITA, Seiji	Technical Associate
NAKANO, Michiko	Technical Associate
SAITO, Midori	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 600, and JNM-LA500), 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), NMR spectrometers (JEOL JNM-ECA920 and JNM-ECS400). In the Myodaiji campus, the following instrument are installed: Electron spin resonance (ESR) spectrometers (Bruker E680, E500, EMX Plus), superconducting quantum interference devices (SQUID; Quantum Design MPMS-7 and MPMS-XL7), powder X-ray diffractometer (MAC Science MXP3), and 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 spectrophotometer (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), 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 2012, Instrument Center accepted more than 90 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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TAKADA, Noriko	Technical Associate
SUGITO,Shouji	Technical Fellow
WADA, Terumi	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 three work sections, mechanics, electronics and glass works 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.

Fabrication of Ellipsoidal Reflector for Inverse Photoelectron Spectroscopy

We have successfully fabricated the Ellipsoidal Reflector for Inverse Photoelectron Spectroscopy as shown in Figure 1. The surface of this mirror should have a form accuracy of 1 μm and high precision a roughness of 10 nm, because it is used for collecting ultraviolet light. For a fabrication with a lower precision level, a CNC Turning Center or Machining Center is used. After the machining, mirror surface with less than R_a 100 μm surface roughness is obtained by hand lapping. However, in this case, a high precision machining is needed. So we fabricated it using the High Precision Turning Machine at National Astronomical Observatory of Japan. The mirror has an asymmetric structure with some holes, which are used to set samples and irradiate electron beam. It was expected that this structure would cause a vibration during the machining and consequently degradations of the form accuracy and the surface state. To avoid this, we worked with an extremely low rotation speed. As a result, the mirror surface with a roughness of R_a 5.8 nm could be successfully obtained as shown in Figure 2.

Figure 1. Ellipsoidal Reflector for Inverse Photoelectron Spectroscopy.

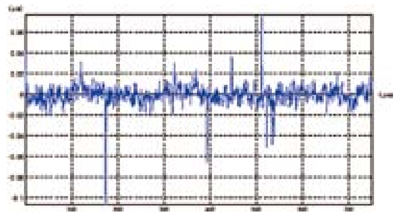

Figure 2. Surface roughness of Ellipsoidal Reflector measured with Laser Probe 3D Measuring Instrument.

Development of Two-Step High Voltage Pulse Generator with the Fast Rise Time

We have developed a two-step high voltage pulse generator having nanoseconds rise time, which is required for the generation of electric fields in time-of-flight mass spectrometry measurements. Figure 3 shows the simplified circuit schematic of the design. The pulse generator is composed of two set of adjustable high voltage power supply and high speed, high voltage switch. The control signals for these high voltage switches are derived from two monostable multivibrator circuits. The apparatus provides a negative step pulse with maximum amplitude of –500 V and a positive step pulse with maximum amplitude of 4.5 kV continuously. The negative pulse width is adjustable from 650 ns to 6 μs, and the positive pulse width is variable from 5 μs to 50 μs. A typical output voltage pulse waveform is shown in Figure 4.

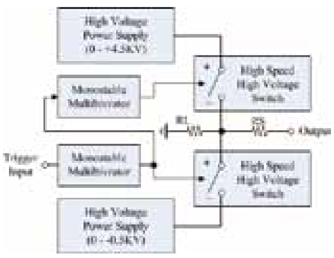

Figure 3. Circuit schematic of the two-step high voltage pulse generator.

Figure 4. Input and Output pulse waveform.

Research Center for Computational Science

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KIM, Kang	Assistant Professor
FUKUDA, Ryoichi	Assistant Professor
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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 (since March 2013), SGI UV1000 (until March 2013) and UV2000 (since April 2013), and Hitachi SR16000 (until February 2013). Over 730 users in 182 project groups from a wide range of molecular science have used in 2012. Large scale calculations, for example the formation of fullerenes, conformation searches using non-Boltzmann sampling methods, and nonlinear spectroscopy of liquids, have been performed with the systems. The Center also provides a number of application programs, for example including 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 2009, contains 125,646 data of quantum chemical studies. Detailed information on the hardware and software at the Center 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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KUWAJIMA, Kunihiro	Professor
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YOSHIOKA, Shiro	Assistant Professor
YAMAGUCHI, Takumi	Assistant Professor
NAKAMURA, Takashi	IMS Research Assistant Professor
SAWAI, Hitomi	IMS Research Assistant Professor
MURAKI, Norifumi	IMS Research Assistant Professor
CHEN, Jin	OIIB 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. The research groups of three full professors and one associate professor who have the position in IMS join OIIB. The research activities of these groups are as follows.

Aono group is studying the bioinorganic chemistry of hemeproteins 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 HrtR that is an heme-sensing transcriptional regulator responsible for heme homeostasis in *Lactococcus lactis*. Kato group is studying structure, dynamics, and interactions of biological macromolecules using nuclear magnetic resonance (NMR) spectroscopy 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 determined quaternary structures of proteasome activators, revealed protein recognition modes of molecular chaperones, and characterized specific interactions of glycolipids with antibacterial peptides and intrinsically disordered proteins. Kuwajima group is studying mechanisms of *in vitro* protein folding and mechanisms of molecular chaperone function. Their goals are to elucidate the physical principles by which a protein organizes its specific native structure from the amino acid sequence. In this year, they studied molecular mechanisms of the cytotoxicity of human α-lactalbumin made lethal to tumor cells (HAMLET) and other protein-oleic acid complexes, in which a protein folding intermediate forms a complex with oleic acid, and this complex has a unique apoptotic activity for the selective killing of tumor cells. 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.

OIIB is conducting the research program, “Integrated Bioscience to Reveal the Entire Life System with Studies of Biofunctional Molecules” and “Research on the Molecular Mechanisms of Biological Responses toward Environmental- and Biological-molecules.” In these research programs, the studies on the following subjects have been carried out: (i) functional analyses of higher-ordered biological phenomena, (ii) comprehensive screening of biofunctional molecules, (iii) computer simulations of higher-ordered biological systems and biofunctional molecules, (iv) molecular mechanisms of response to environmental molecules, of differentiation of germ cells, and of cellular stress-response and defense against stress, (v) studies on perturbation of biological functions induced by environmental molecules, (vi) studies on normal physiological functions regulated by biological molecules, and (vii) construction of integrated data base on the biological influences of environmental molecules.

Safety Office

UOZUMI, Yasuhiro	Director
TOMURA, Masaaki	Assistant Professor
TANAKA, Shoji	Assistant Professor
SUZUI, Mitsukazu	Technical Associate
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.