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 (1978–2016).

UVSOR Synchrotron Facility

KOSUGI, Nobuhiro	Director, Professor
KATOH, Masahiro	Professor
SHIGEMASA, Eiji	Associate Professor
TANAKA, Kiyohisa	Associate Professor
IWAYAMA, Hiroshi	Assistant Professor
OHIGASHI, Takuji	Assistant Professor
IDETA, Shin-ichiro	Assistant Professor
FUJIMOTO, Masaki	Assistant Professor
NAKAMURA, Eiken	Technical Assosiate
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
YANO, Takayuki	Technical Associate
INAGAKI, Yuichi	Technical Associate
HORIGOME, Toshio	Administrative Associate
TOKUSHI, Tetsujou	Technical Fellow
HAYASHI, Ken-ichi	Technical Fellow
MINAKUCHI, Aki	Technical Fellow
HAGIWARA, Hisayo	Secretary
INAGAKI, Itsuko	Secretary

Outline of the UVSOR Synchrotron Facility

Since the first light in 1983, UVSOR Synchrotron Facility has been successfully operated as one of the major synchrotron light sources in Japan. After the major upgrade of the accelerators in 2003, UVSOR Synchrotron was renamed to UVSOR-II Synchrotron and became one of the world's brightest low energy synchrotron light sources. In 2012, it was upgraded again and has been renamed to be UVSOR-III Synchrotron. The brightness of the electron beam was increased further. Today, six undulators are installed in total, and the storage ring is regularly operated in the top-up mode, in which the electron beam current is kept constant, irrespective of multi (16) bunches or single bunch.

The UVSOR accelerator complex consists of a 15 MeV injector linac, a 0.75 GeV booster synchrotron, and a 0.75 GeV 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 top-up operation for time-resolved measurements or low current measurements is also conducted for two weeks per year.

Six undulators and eight bending magnets provide synchrotron radiation (SR). The bending magnet, its radius of 2.2 m, produces SR with the critical energy of 425 eV. There are eight bending magnet beamlines (BL1B–BL7B, and BL2A to be moved to BL8B). Three of the six undulators are in-vacuum soft X-ray (SX) linear-polarized undulators (BL3U, BL4U, BL6U) and the other three are vacuum/extreme ultraviolet (VUV/XUV or EUV) circular-polarized undulators (BL1U, BL5U, BL7U). In total, fourteen beamlines (= fourteen endstations) are now operating in two categories: Twelve are so-called "public beamlines," which are open to scientists from universities, governmental research institutes, public and private enterprises, and also to overseas scientists; the other two beamlines are so-called "in-house beamlines," which are dedicated to strategic projects conducted by internal IMS groups in tight collaboration with domestic and foreign scientists. From the viewpoint of photon energies, we have 1 SX station equipped with a double-crystal monochromator, 7 SX stations with a grazing incidence monochromator, 3 VUV stations with a normal incidence monochromator, 2 infrared/tera Hz stations equipped with Fourier transform interferometers and 1 beamline for light source development without any monochromators.

Figure 1. UVSOR-III electron storage ring, radiation shield wall, and beamlines/endstations.

Inter-University and International Collaboration Programs

A variety of molecular science and related subjects have been carried out at UVSOR Synchrotron by IMS and external/overseas researchers. The number of visiting researchers per year tops > 1200, who come from > 60 different institutes. International collaboration is also pursued actively, and the number of visiting foreign researchers reaches >100 from >10 countries. UVSOR-III Synchrotron invites new/continuing research proposals twice a year. The proposals both for academic and public research (charge-free) and for private enterprises (charged) are acceptable. The fruits of the research activities using UVSOR-III Synchrotron are published as the UVSOR ACTIVITY REPORT annually.

Recent Developments

BL6B is an Infrared-THz beamline which has confocal type micro-spectroscope station, reflection/transmission station, and IR microscope imaging station. To solve serious long term drift of beam path caused by M0 magic mirror thermal load, the feedback control system of M0 mirror angle by monitoring the reflection of visible laser light from M0 mirror has been developed. This feedback control system has been routinely operated and successfully provides stable beam for users from this year.

Reserch Highlights[1)]

Optical vortex has a helical wavefront and carries orbital angular momentum (OAM) as well as spin angular momentum associated with its circular polarization. Differing from plane-wave photons, violation of the standard electric dipole selection rules is predicted in an interaction between the optical vortex and an atom, as a consequence of the transference of the OAM to the internal degrees of freedom of the atom. The experiment on vortex-matter interactions in the VUV energy range was carried out for the first time, at the beamline BL1U. The VUV vortex beams at about 30 eV photon energy were produced by a helical undulator as the higher harmonics. Photoelectron angular distributions of helium atoms were measured by using a velocity map imaging spectrometer. Figure 1 shows the angular distributions measured for the first, second and third harmonics, corresponding to plane-wave photons ($l = 0$), and VUV vortices of $l = 1$ and 2, respectively. While the violation of the electric dipole transition rules has been predicted for interactions between vortices and atoms, the photoelectron angular distributions are well reproduced by the dipole components alone, and non-dipole contributions are not detected within the experimental uncertainty. This observation can be explained by the localized nature of the helical phase effect of the vortex on the interaction with atoms, and demonstrates that non-dipole interactions induced by vortex are hardly observable in conventional gas-phase experiments.

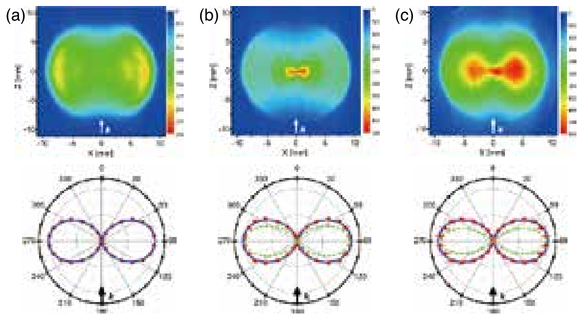


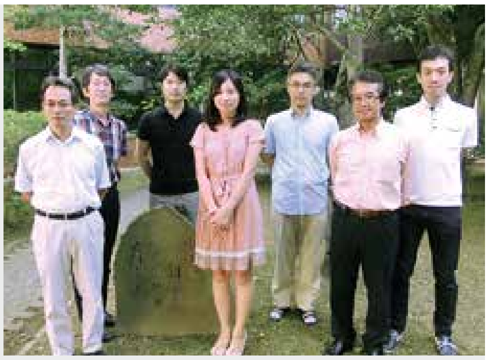
Figure 2. Photoelectron angular distributions of helium atoms measured for the (a) first, (b) second and (c) third harmonics from helical undulator. The solid blue curves represent fits assuming electric dipole transition. The dotted green curves in (b) and (c) show the angular dependence of the photoelectron expected for non-dipole transitions induced by the OAM carried by the VUV vortex.

Reference

1) T. Kaneyasu *et al.*, *Phys. Rev. A* **95**, 023413 (2017).

Center for Mesoscopic Sciences

OKAMOTO, Hiromi	Director, Professor
OHMORI, Kenji	Professor
IINO, Ryota	Professor
TAIRA, Takunori	Associate Professor
FUJI, Takao	Associate Professor
NOBUSADA, Katsuyuki	Associate Professor
NARUSHIMA, Tetsuya	Assistant Professor
YOSHIZAWA, Daichi	Assistant Professor
ISHIZUKI, Hideki	Assistant Professor
NOMURA, Yutaka	Assistant Professor
SHIRAI, Hideto	IMS Research Assistant Professor
OKANO, Yasuaki	Technical Associate
MASUDA, Michiko	Secretary
NOMURA, Emiko	Secretary



As the succeeding organization of former Laser Research Center for Molecular Science, Center for Mesoscopic Sciences continues development of new experimental apparatus and methods to open groundbreaking research fields in molecular science, in collaboration with other departments and facilities. Those new apparatus and methods will be served as key resources in advanced collaboration with the researchers from the community of molecular science. The targets cover:

- advanced photon sources ranging from terahertz to soft X-ray regions
- novel quantum-control schemes based on intense and ultrafast lasers
- novel optical imaging and nanometric microscopy

and so forth.

The Center also possesses several general-purpose instruments for laser-related measurements (commercial as well as in-house developed), and lends them to researchers in IMS who conduct laser-based studies, so as to support and contribute to their advanced researches.

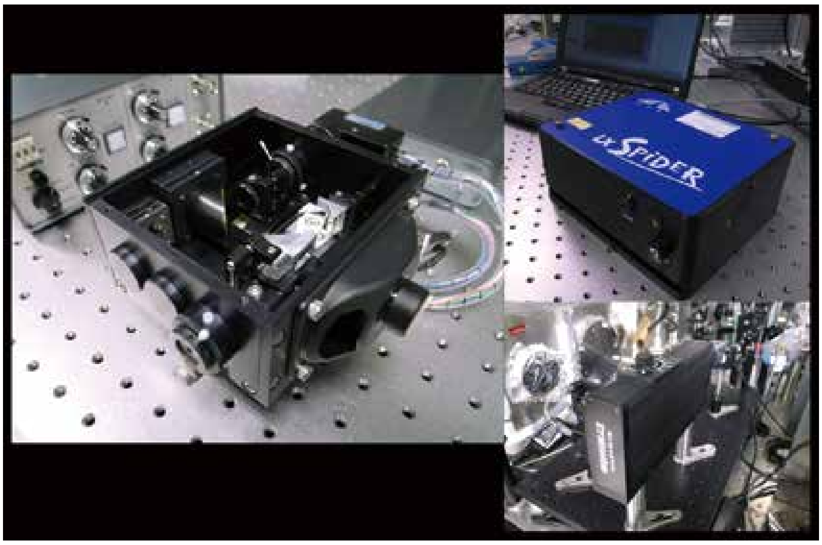


Figure 1. (left) A Fringe-Resolved Autocorrelation (FRAC) apparatus for sub-10 fs pulse characterization designed in the Center. (upper right) Spectral Phase Interferometry for Direct Electric-Field Reconstruction (SPIDER) and (lower right) Frequency-Resolved Optical Gating (FROG) apparatuses for general-purpose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

Instrument Center

KERA, Satoshi	Director, Professor
YOKOYAMA, Toshihiko	Professor
TAKAYAMA, Takashi	Technical Associate
FUJIWARA, Motoyasu	Technical Associate
OKANO, Yoshinori	Technical Associate
MIZUKAWA, Tetsunori	Technical Associate
MAKITA, Seiji	Technical Associate
UEDA, Tadashi	Technical Associate
OHARA, Mika	Nano. Platform Manager
AZUMA, Yosuke	Nano. Platform Manager
NODA, Ippei	Nano. Platform Coordinator
NAKAO, Satoru	Post-Doctoral Fellow
NAGAO, Haruyo	Technical Fellow
IKI, Shinako	Technical Fellow
MATSUO, Yukiko	Technical Fellow
FUJIKAWA, Kiyoe	Technical Fellow
OTA, Akiyo	Secretary
YOKOTA, Mitsuyo	Secretary
FUNAKI, Yumiko	Secretary
HYODO, Yumiko	Secretary
TOYAMA, Yu	Secretary
IWANO, Yukie	Secretary

Instrument Center was organized in April of 2007 by integrating the general-purpose and state-of-the-art 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 researches by utilizing general-purpose and state-of-the-art instruments. The staffs of Instrument Center maintain the best conditions 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 (JNM-ECA 600 for solutions, JNM-ECS400 for solutions and Bruker AVANCE800 Cryoprobe for solutions), matrix assisted laser desorption/ionization time-of-flight (MALDI TOF) mass spectrometer (Voyager DESTR), 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), focused ion beam (FIB) processing machine (JEOL JEM-9310FIB), and 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 for solids), superconducting quantum interference devices (SQUID; Quantum Design MPMS-7 and MPMS-XL7), 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 spectrometer (SPEX Fluorolog2), X-ray fluorescence spectrometer (JEOL JSX-3400RII), UV-VIS-NIR spectrometer (Hitachi U-3500), Raman microscope (Renishaw INVIA REFLEX 532), nanosecond excimer/dye laser system (Lambda Physics LPX105i/LPD3002), Nd:YAG pumped OPO laser (Spectra Physics GCR-250/Lambda Physics Scanmate OPPO), fluorinated excimer laser (Lambda Physics Complex 110F), picosecond tunable laser system (Spectra Physics Tsunami/ Quantronix Titan/Light Conversion TOPAS), low vacuum analytical SEM (Hitachi SU6600), electron spectrometers for chemical analysis (ESCA) (Omicron EA-125), angle resolved ultraviolet photoelectron spectroscopy (ARUPS) for functional band structures (VG-Scienta DA30), and FTIR spectrometer (Bruker IFS 66v/S). In the fiscal year of 2016, Instrument Center accepted 105 applications from institutions outside IMS and the total user time including in-house use amounted 2,926 days/36 equipments. Instrument Center also maintains helium liquefiers in the both campus and provides liquid helium to users (62,320 L/year). Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute (41,434 L/year). The staffs of Instrument Center provide consultation for how to treat liquid helium, and provide various parts necessary for low-temperature experiments.

Instrument Center organizes the Inter-University Network for Common Utilization of Research Equipments and the Molecule and Material Synthesis Platform in the Nanotechnology Platform Program supported by Ministry of Education, Culture, Sports, Science and Technology. These special programs are described in the other chapter of the booklet.

Equipment Development Center

YAMAMOTO, Hiroshi	Director
MIZUTANI, Nobuo	Technical Associate
AOYAMA, Masaki	Technical Associate
KONDOU, Takuhiko	Technical Associate
TOYODA, Tomonori	Technical Associate
TAKADA, Noriko	Technical Associate
NAKANO, Michiko	Technical Associate
KIMURA, Sachiyo	Specially Appointed Technical Associate
KOSUGI, Yuta	Specially Appointed Technical Associate
TANAKA,Takashi	Technical Fellow
SAWADA, Toshihiro	Technical Fellow
YOSHIDA, Hisashi	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.

Development of Microfluidic Channel with a Step Structure by Lithography

We have developed a microfluidic channel with a step structure, which has depth of 50 μm and 1 μm, and width of 300 μm, on 70×30(mm) glass substrate by wet etching. We expect the structure to improve the efficiency of chemical reaction by limiting depth of reaction part.

Since it is not able to fabricate different depth structures by a single etching process in lithography, we need to repeat the process for each depth pattern. First, we created a channel with 50 μm depth. Next, we added 1 μm depth structure with precise position aligning. We examined etching solutions, mask materials suitable for each etching depth, roughness of resist surface, and alignment procedures. With these investigations, a step structure whose profile is shown in Figure 1 has been obtained.

High Voltage Amplifier for Driving Bimorph Pump

In order to flow very little amount of solution by using a bimorph pump that is driven by AC voltage, an embedded power supply is normally used. However, since it is difficult to adjust the output voltage, there is a problem of low reproducibility at experiments. In addition, since the cable connection is easily disconnected, troubles such as short circuit are likely to occur. We have developed high voltage amplifier for driving bimorph pump with high reproducibility and safety. It is shown in Figure 2.

First, AD9834BRUZ DDS (Direct Digital Synthesizer; Analog Devices), generates a sine wave whose amplitude is 3.5Vp-p and frequency is from 10 Hz to 100 Hz with resolution of 1 Hz. Next, ADA4077-1ARZ (Analog Devices) amplifies the fed signal by 4 times, to be followed by another amplification by ADA4077-1ARZ and AD5292BRUZ (Analog Devices) at a ratio ranging from 0 to −1. Finally, PA441DF (APEX) amplifies the signal to ±140 V. All devices are operated by ARM microcontroller LPC1114FBD48/302 (NXP) through SPI (Serial Peripheral Interface). The values are displayed on OLED screen and recorded in EEPROM.

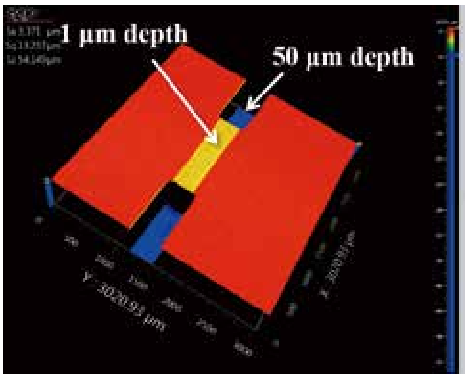


Figure 1. 3D view of the microfluidic channel with a step structure.

Figure 2. High voltage amplifier for driving bimorph pump.

Research Center for Computational Science

SAITO, Shinji	Director, Professor
EHARA, Masahiro	Professor
OKUMURA, Hisashi	Associate Professor
OONO, Hitoshi	Assistant Professor
ISHIDA, Tateki	Assistant Professor
ITOH, Satoru G.	Assistant Professor
ITO, Soichi	Assistant Professor
MIZUTANI, Fumiyasu	Technical Associate
IWAHASHI, Kensuke	Technical Associate
NAITO, Shigeki	Technical Associate
SAWA, Masataka	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.* solid state physics and biophysics. The computer systems consist of Fujitsu PRIMERGY RX300, PRIME HPC FX10 and PRIMERGY CX2550, SGI UV2000. The systems have been used by 813 people in 221 research groups in 2016. Large scale calculations, for example accurate electronic structure calculations of molecular systems and conformation searches using non-Boltzmann ensemble methods, 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 members of the Center. The latest release, QCLDB II Release 2016, contains 139,657 data of quantum chemical studies. Detailed information on the hardware and software is available on the web site (http://ccportal.ims.ac.jp/).

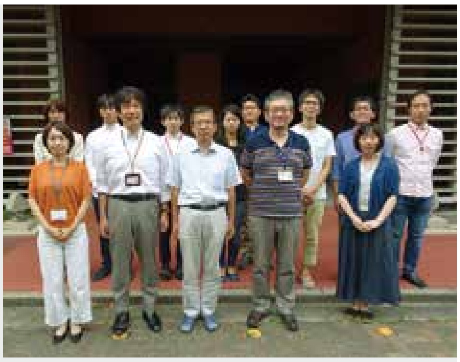
In addition to the provision of computational resources to individual academic researchers in Japan, the Center contributes up to 20% of the computational resources to the Post-K Supercomputer Priority Researches 5 and 7 and the Professional development Consortium for Computational Materials Scientists.

Figure 1. Fujitsu PRIMERGY CX2550.

Figure 2. SGI UV2000.

Okazaki Institute for Integrative Bioscience

AONO, Shigetoshi	Professor
KATO, Koichi	Professor
IINO, Ryota	Professor
KURIHARA, Kensuke	Research Associate Professor
KURAHASHI, Takuya	Assistant Professor
YOSHIOKA, Shiro	Assistant Professor
NAKAMURA, Akihiko	Assistant Professor
MURAKI, Norifumi	Assistant Professor
YAGI-UTSUMI, Maho	Assistant Professor
ANDO, Jun	Assistant Professor
YANAKA, Saeko	IMS Research Assistant Professor
TANAKA, Kei	Secretary
NAKANE, Kaori	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. Their research interests are focused on the structure and function relationships of transcriptional regulators and metal transport proteins that are responsible for metal homeostasis, especially iron and/or heme homeostasis, in bacteria. They are also working on a novel photosensor protein that adopts vitamin B_{12} (adenosylcobalamin) as the active site for photosensing, which is a transcriptional factor regulating gene expression in response to visible ligth. They successfully determined the crystal structures of HtaA, HtaB, and HmuT that are heme-binding and heme-transport proteins responsible for heme uptake reaction in *Croynebacterium glutamicum*. They also determined the crystal structure of a novel photosensor protein CarH from *Thermus thermophilus*, which uses adenosylcobalamin as a photoreceptor. Iino group is studying operation and design principles of molecular machines using single-molecule analysis, structural analysis, and protein engineering. Especially, they focus on rotary and linear molecular motors. In this year, they have succeeded in direct observation of 1-nm stepping motion of a linear molecular motor chitinase A moving on crystalline chitin. They also have revealed that chitinase A operates as the Brownian ratchet, and decrystallization of single polymer chain from the crystal is the rate-limiting step of the processive movement of chitinase A. Furthermore, as protein engineering approach, they have determined the crystal structures of computationally redesigned functional chitinase A molecules. 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 characterized conformational dynamics of a high-mannose-type oligosaccharide with a critical determinant recognized by molecular chaperones and also created self-assembled glycoclusters exhibiting homophilic hyper-assembly in a Ca^{2+}-dependent manner through specific carbohydrate–carbohydrate interactions. Kurihara group is studying artificial chemical cells consisted of supramolecular assemblies, *e.g.* vesicle, oil droplet. Their goal is to create artificial cells which has three main elements: Information, compartment and metabolism (protein). They achieved the self-reproducing oil droplet system, which lead to the formation of giant vesicular compartment. In this year, by developing the self-reproducing oil droplet system, they are constructing vesicular system containing oligopeptides which are spontaneously generated by native chemical ligations.

Safety Office

UOZUMI, Yasuhiro	Director
TOMURA, Masaaki	Assistant Professor
TANAKA, Shoji	Assistant Professor
SUZUI, Mitsukazu	Technical Associate
UEDA, Tadashi	Technical Associate
TAKAYAMA, Takashi	Technical Associate
SAKAI, Masahiro	Technical Associate
MAKITA, Seiji	Technical Associate
KONDO, Naonori	Technical Associate
MIZUTANI, Nobuo	Technical Associate
ONITAKE, Naoko	Secretary
TSURUTA, Yumiko	Secretary
KAMO, Kyoko	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 composed 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.