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 (1978–2017).

UVSOR Synchrotron Facility

KERA, Satoshi	Director, Professor
KATOH, Masahiro	Professor
TANAKA, Kiyohisa	Associate Professor
MATSUI, Fumihiko	Senior Researcher
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
MAKITA,Seiji	Technical Associate
HORIGOME, Toshio	Specially Appointed Technical Associate
YUZAWA, Hayato	Specially Appointed Technical Associate
MINAKUCHI, Aki	Technical Fellow
HAGIWARA, Hisayo	Secretary
INAGAKI, Itsuko	Secretary

Outline of the UVSOR Synchrotron Facility

Since the first light in 1983, the UVSOR Synchrotron Facility has been successfully operated as one of the major synchrotron light sources in Japan. After the major upgrade of 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, that is approximately 50 meters in circumference, is regularly operated in the top-up mode, in which the electron beam current is kept constant, irrespective of multi 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 (Table. 1). Three of the six

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

Table 1. List of beamlines at UVSOR-III Synchrotron.

Beamline	Monochromator / Spectrometer	Energy Range	Targets	Techniques
BL1U	Free electron laser	1.6 - 13.9 eV	Gas Liquid Solid	Irradiation
BL1B	Martin-Puplett FT-FIR	0.5 - 30 meV	Solid	Reflection Absorption
BL2A	Double crystal	585 eV - 4 keV	Solid	Reflection Absorption
BL2B	18-m spherical grating (Dragon)	23 - 205 eV	Solid	Photoemission
BL3U	Varied-line-spacing plane grating (Monk-Gillieson)	60 - 800 eV	Gas Liquid Solid	Absorption Photoemission Photon-emission
BL3B	2.5-m off-plane Eagle	1.7 - 31 eV	Solid	Reflection Absorption
BL4U	Varied-line-spacing plane grating (Monk-Gillieson)	130 - 700 eV	Gas Liquid Solid	Absorption (Microscopy)
BL4B	Varied-line-spacing plane grating (Monk-Gillieson)	25 eV - 1 keV	Gas Solid	Photoionization Photodissociation Photoemission
BL5U	Varied-line-spacing plane grating (Monk-Gillieson)	20 - 200 eV	Solid	Photoemission
BL5B	Plane grating	6 - 600 eV	Solid	Calibration Absorption
BL6U*	Variable-included-angle varied-line-spacing plane grating	40 - 800 eV	Gas Solid	Photoionization Photodissociation Photoemission
BL6B	Michelson FT-IR	4 meV - 2.5 eV	Solid	Reflection Absorption
BL7U	10-m normal incidence (modified Wadsworth)	6 - 40 eV	Solid	Photoemission
BL7B	3-m normal incidence	1.2 - 25 eV	Solid	Reflection Absorption

Yellow columns represent undulator beamlines.
* In-house beamline.

undulators are in- vacuum soft X-ray (SX) linear-polarized undulators (BL3U, BL4U, and BL6U) and the other three are vacuum/extreme ultraviolet (VUV/XUV or EUV) circular-polarized undulators (BL1U, BL5U, and BL7U). In total, fourteen beamlines are now operating and except for BL1U and BL6U they are so-called "public beamlines," which are open to scientists from universities, governmental research institutes, public and private enterprises, and also to overseas scientists. 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. Since 2018, BL1U is partly opened for using as public beamline.

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, two IR/THz stations equipped with Fourier transform interferometers and 1 beamline for light source development without any monochromators.

Inter-University and International Collaboration Programs

A variety of molecular science and related subjects have been carried out at UVSOR Synchrotron Facility by IMS and external/overseas researchers. The number of visiting researchers per year tops > 1200, whose come from > 60 different institutes. International collaboration is also pursued actively, and the number of visiting foreign researchers reaches ~70 from 13 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

A soft X-ray beamline BL5U has been open for users since 2016 and used as high-energy resolution ARPES beamline. By introducing a final focusing mirror close to the sample position (~50 mm), the synchrotron light whose original size was 400 (H) × 120 (V) is successfully focused to 23 (H) × 40 (V) μm. ARPES study on small samples or inhomogeneous samples is now available.

Beamline BL4U has been open for users since 2013 and used as high-resolution X-ray transmission microscopy (STXM). The extension of the photon energy range is demanded to cover much broaden research field. Adopting Fresnel zone plate for low-energy range, we are approaching to get 50 eV which may cover Li K-edge. Although it is challenging how to optimize the optical parameters, BL4U will be an unique and attractive beamline for studying varisou novel materials including solid battery.

The UVSOR accelerators have been operated for more than 30 years. We have been upgrading and replacing the machine components, such as magnet power supplies or RF power amplifiers, to continue the stable operation. In these years, troubles occurred on some core components, such as the vacuum chambers and the magnets. We are carefully planning their replacements with short shutdown periods and under the limitation of the facility budget.

Reserch Highlights[1)]

Understanding the mechanism of charge transfer in functional molecular solids, the electronic structure measurement, especially of the energy-band dispersion, is requested for molecular materials. However the electronic structure measurement has not been well achieved due to experimental difficulties for the molecular solids. More importantly, the dynamic interaction between the traveling charges and the molecular vibrations is critical for the charge transport in organic semiconductors. However, a direct evidence of the expected impact of the charge–phonon coupling on the band dispersion of organic semiconductors is yet to be provided. We reported on the electronic properties of rubrene single crystal as investigated by angle resolved ultraviolet photoelectron spectroscopy using low-excitation photon energy. A gap opening and kink-like features in the rubrene electronic band dispersion are observed thanks to high-energy and momentum resolutions in BL7U. In particular, the latter results in a large enhancement of the hole effective mass, well above the limit of the theoretical estimations. The results are consistent with the expected modifications of the band structures in organic semiconductors as introduced by hole–phonon coupling effects and represent an important experimental step toward the understanding of the charge localization phenomena in organic materials.

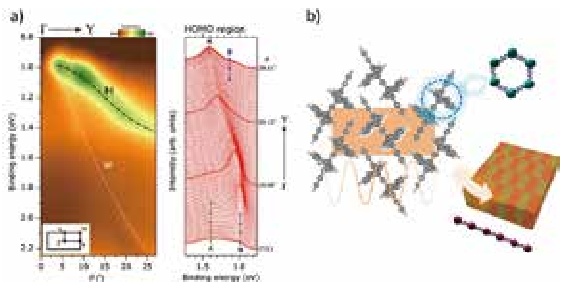

Figure 2. Renormalization of the energy-band dispersion of highest-occupied molecular orbital (HOMO) band of rubrene single crystal at 300 K by coupling collective phonons and intramolecular vibrations. a) Angle-resolved photoelectron spectra recorded along ΓY direction of the single crystal. The intensity map as a function of the emission angle θ is also shown (left). The HOMO (H) dispersion is indicated by dash dotted black curve as guides for the eye. The feature W due to secondary electron emission which reflects the density of states and band dispersion of unoccupied states is superimposed. b) Schematic of the molecular orientation in the crystalline a-b plane of rubrene single crystal. Images of collective phonon in the crystal and local intramolecular vibration are also shown.

Reference

1) F. Bussolotti *et al.*, *Nat. Commun.* **8**, 173–179 (2017).

Center for Mesoscopic Sciences

OKAMOTO, Hiromi	Director, Professor
OHMORI, Kenji	Professor
IINO, Ryota	Professor
TAIRA, Takunori	Associate Professor
FUJI, Takao	Associate Professor
(the late) NOBUSADA, Katsuyuki	Associate Professor
SUGIMOTO, Toshiki	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.

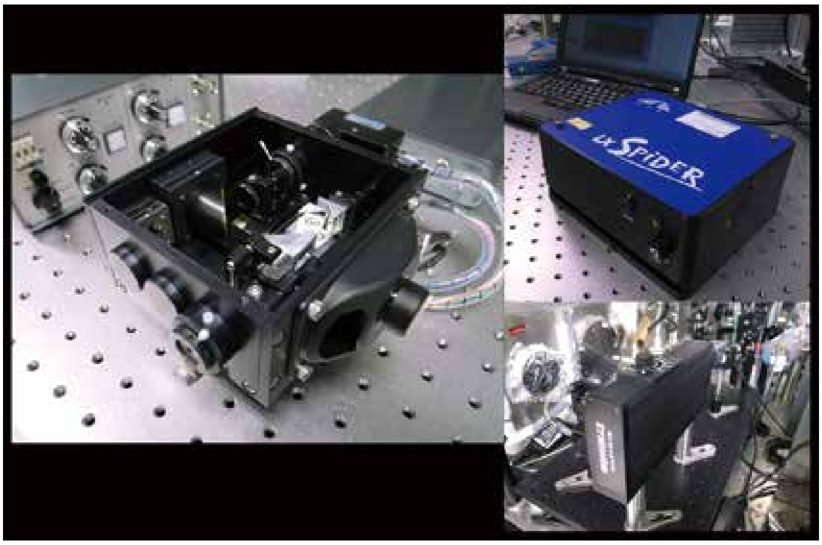

Figure 1. (left) A Fringe-Resolved Autocorrelation (FRAC) apparatus for sub-10 fs pulse characterization designed in the Center. (upper right) Spectral Phase Interferometry for Direct Electric-Field Reconstruction (SPIDER) and (lower right) Frequency-Resolved Optical Gating (FROG) apparatuses for general-purpose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

Instrument Center

YOKOYAMA, Toshihiko	Director, Professor
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OKANO, Yoshinori	Technical Associate
MIZUKAWA, Tetsunori	Technical Associate
UEDA, Tadashi	Technical Associate
OHARA, Mika	Nano. Platform Manager
HIGASHI, 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
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IWANO, Yukie	Secretary
SHIBATA, Yuka	Secretary
ITO, Sumie	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 (microflex LRF, Bruker Daltonics), powder X-ray diffractometer (Rigaku RINT-Ultima III), circular dichroism (CD) spectrometer (JASCO JW-720WI), differential scanning calorimeter (MicroCal VP-DSC), isothermal titration calorimeter (MicroCal iTC200), solid-state calorimeter (Rigaku DSC8231/TG-DTA8122), 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 2017, Instrument Center accepted 115 applications from outside and the total user time amounted 2,483 days for outside and 748 days for in-house with 34 equipments. Instrument Center also maintains helium liquefiers in the both campus and provides liquid helium to users (53,622 L/year). Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute (41,042 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

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AOYAMA, Masaki	Technical Associate
KONDOU, Takuhiko	Technical Associate
TOYODA, Tomonori	Technical Associate
TAKADA, Noriko	Technical Associate
NAKANO, Michiko	Technical Associate
KIMURA, Sachiyo	Technical Associate
KIKUCHI, Takuro	Specially Appointed Technical Associate
KIMURA, Kazunori	Specially Appointed Technical Associate
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 a Special Shape Coil

We are developing a special shape electromagnetic coil that can generate rotating magnetic field inside a cavity. This rotating filed is important for aligning particles dispersed in a liquid. Since the shape and arrangement of coils affect the flow of magnetic flux with large complexity, it is not easy to estimate the direction and strength of magnetic flux generated by the coils. Therefore, computer-aided engineering is very important to help the designing. At the same time, we are fabricating the prototype model and evaluating the flow of magnetic flux by comparing the simulation and measurement result.

First, we have fabricated a winding machine to roll up wires in a customized way. Next, we have fabricated a simple shaped coil (wire diameter 0.6 mm, 725 turns), and measured generated magnetic flux density by a Gauss meter. As the result of comparison between the results of simulation and experiments, a good matching was confirmed. (Figure 1)

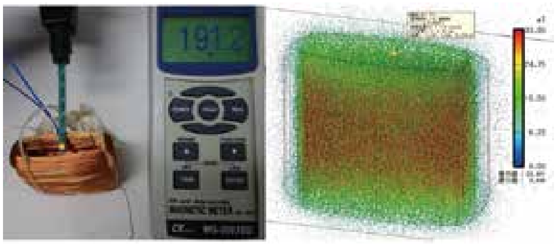

Figure 1. Measurement of magnetic flux density generated in a coil and result of CAE: 191.2 Gauss on experiment, 192 Gauss on CAE.

Now, we are not only optimizing the shape and material of the coil, but also developing a novel fabrication method for a special shaped coil.

Signal Fan-Out Buffer and Distributor

When we distribute a signal from photo diode/MCP/Photo-Multiplier Tube (PMT) to an oscilloscope or a data acquisition system, we normally use BNC T type adapter and coaxial cable. However, such connections cause huge attenuation and/or degradation of the signal.

Our Signal Fan-out buffer and Distributor (SFD) can output copied input signal (up to ±5V, 20 MHz) to multiple channels (up to 8), and can prevent degradation of signal using driving circuit by THS3001ID (Texas Instruments). In addition, SFD indicates, by two-color LED, the polarity of input/output signals, as well as connection/ disconnection of cables using unique detection circuit by JFET operational amplifier ADA4610-2ARZ (Analog Devices). By the latter function, the users can grasp unexpected dropouts and disconnections of cables visually.

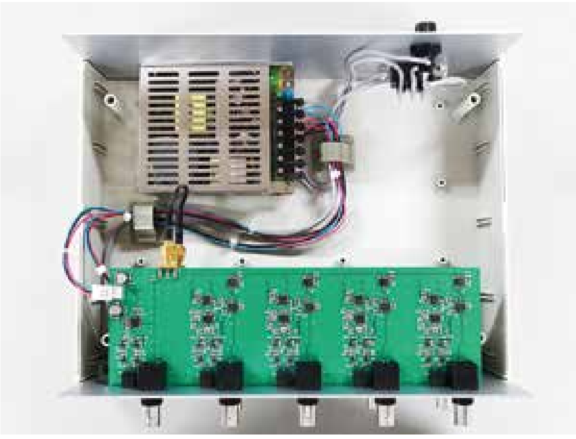

Figure 2. Inside view of Signal Fan-out Buffer and Distributor.

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
UCHIYAMA, Ikuo	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
KAMIYA, Motoshi	Specially Appointed Technical Associate
TOYA, Akiko	Secretary
ISHIHARA, Mayumi	Secretary
KONDO, Naoko	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, biophysics, and physiology. Our systems consist of NEC LX (406Rh-2, 110-Rh1, 108Th-4G; since Oct. 2017), Fujitsu PRIME HPC FX10, Fujitsu PRIMERGY (RX300 and CX2550; until Sep. 2017), and SGI UV2000 (until Sep. 2017). The NEC LX 406Rh-2 and 110-Rh1 combined system, named "Molecular Simulator," is ranked 93rd position in the TOP500 supercomputer list in June 2018. These massive computer resources have been used for various kinds of large-scale calculations, for example accurate electronic structure calculations of molecular systems and conformation searches using non-Boltzmann ensemble methods. We also provide a number of application programs to the users: Gaussian, GAMESS, Molpro, AMBER, Gromacs, and so on. The supercomputer systems had been used by 837 researchers from 224 groups in fiscal year 2017. Some of the computational resources are provided to the following projects: Post-K Supercomputer Priority Issues 5 and 7, Post-K Exploratory Challenge: Challenge of Basic Science—Exploring Extremes through Multi-Physics and Multi-Scale Simulations, Professional development Consortium for Computational Materials Scientists (PCoMS), and Elementary Strategy Initiative to Form a Core Research Center.

We also offer Quantum Chemistry Literature Database (QCLDB; http://qcldb2.ims.ac.jp/), Force Constant Database (FCDB; http://fcdb.ims.ac.jp/), and Segmented Gaussian Basis Set (SGBS; http://sapporo.center.ims.ac.jp/sapporo/) services. QCLDB had been developed by the Quantum Chemistry Database Group in collaboration with members of the center. The latest release, QCLDB II Release 2016, containing 139,657 data of quantum chemical studies is available for the registered users. FCDB provides force constants of molecules collected from literature, which are very important physical properties in vibrational spectrum analyses. SGBS service provides basis sets for atoms which efficiently incorporate valence and core electron correlations (also known as Sapporo basis sets) in various quantum chemistry package formats. Further details about the hardware, software, and the other services are available on our website (English: https://ccportal.ims.ac.jp/en/, Japanese: https://ccportal.ims.ac.jp/).

Figure 1. NEC LX.

Figure 2. Fujitsu PRIME HPC FX10.

Safety Office

UOZUMI, Yasuhiro	Director
TOMURA, Masaaki	Assistant Professor
TANAKA, Shoji	Assistant Professor
SHIGEMASA, Eiji	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
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.