RESEARCH FACILITIES

The Institute includes four research facilities, UVSOR Synchrotron Facility, Instrument Center, Equipment Development Center, and Research Center for Computational Science (Okazaki Research Facilities).

UVSOR Synchrotron Facility

KERA, Satoshi	Director, Professor
MATSUI, Fumihiko	Professor
KATOH, Masahiro	Project Professor (Hiroshima Univ.)
TANAKA, Kiyohisa	Associate Professor
TAIRA, Yoshitaka	Associate Professor
OHIGASHI, Takuji	Associate Professor (Cross Appt.)
KANEYASU, Tatsuo	Associate Professor (SAGA-LS)
ARAKI, Tohru	Senior Researcher
IWAYAMA, Hiroshi	Assistant Professor
SUGITA, Kento	Assistant Professor
KATAYANAGI, Hideki	Research Associate
HAGIWARA, Kenta	IMS Fellow
MATSUDA, Hiroyuki	Post-Doctoral Fellow
SALEHI, Elham	Post-Doctoral Fellow
HAYASHI, Kenji	Engineer (Unit Leader)
NAKAMURA, Eiken	Chief Engineer
MAKITA,Seiji	Engineer
SAKAI, Masahiro	Chief Technician
YANO, Takayuki	Chief Technician
OKANO, Yasuaki	Chief Technician
TESHIMA, Fumitsuna	Chief Technician
KONDO, Naonori	Chief Technician
YUZAWA, Hayato	Chief Technician
OTA, Hiroshi	Technician
SHIMIZU, Kohei	Technician
HORIGOME, Toshio	Technical Fellow
MINAKUCHI, Aki	Technical Fellow
MIZUKAWA, Tetsunori	Technical Fellow
SUGIMOTO, Yasunobu	Technical Fellow
YAMAZAKI, Jun-ichiro	Technical Fellow
ISHIHARA, Mayumi	Secretary
KAMO, Kyoko	Secretary
YOKOTA, Mitsuyo	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 *ca.* 53 meters in circumference, is regularly operated in the top-up mode, 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 single bunch top-up operation (176 ns, 5.6 MHz) 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 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). Two beamlines, BL1U and BL6U, 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. Other twelve beamlines are so-called "public beamlines," which are open to scientists from universities, governmental research institutes, public and private enterprises, and also to overseas scientists. After each development, the in-house beamline will be opened for use as a public beamline.

From the viewpoint of photon energies, we have one SX station equipped with a double-crystal monochromator, seven SX stations with a grazing incidence monochromator, three VUV stations with a normal incidence monochromator, two IR/THz stations equipped with Fourier transform interferometers and one beamline for light source development without any monochromators.

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

Beamline	Optics	Energy Range	Targets	Techniques
BL1B	Martin-Puplett FT-FIR	0.5-30 meV	Solid	Reflection/Adsorption
BL6B	Michelson FT-IR	4 meV-2.5 eV	Solid	Reflection/Adsorption
BL7B	3-m normal incidence	1.2-25 eV	Solid	Reflection/Adsorption
BL3B	2.5-m off-plane Eagle	1.7-31 eV	Solid	Reflection/Absorption
BL5B	Plane grating	6-600 eV	Solid	Calibration/Absorption
BL2B	18-m spherical grating (Dragon)	23-205 eV	Solid	Photoionization Photodissociation
BL4B	Varied-line-spacing plane grating (Monk-Gillieson)	25 eV-1 keV	Gas, Liq. Solid	Photoionization, XAFS Photodissociation, XMCD
BL2A	Double crystal	585 eV-4 keV	Solid	Reflection/XAFS
BL1U	Tandem undulators/ Free electron laser	1.6-13.9 eV	Gas Solid	Laser Compton Scattering Orbital Momentum Light
BL7U	10-m normal incidence (modified Wadsworth)	6-40 eV	Solid	Photoemission
BL5U	Varied-line-spacing plane grating (Monk-Gillieson)	20-200 eV	Solid	ARPES Spin-resolved ARPES
BL6U	Variable-inc.-angle-varied-line-spacing plane grating	40-700 eV	Solid	ARPES XAFS / XPD
BL4U	Varied-line-spacing plane grating (Monk-Gillieson)	50-700 eV	Gas, Liq. Solid	XAFS Microscopy (STXM)
BL3U	Varied-line-spacing plane grating (Monk-Gillieson)	60-800 eV	Gas, Liq. Solid	XAFS / Photoemission Photon-emission

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 cumulative total number of visiting researchers (person-days) per year tops > 5000, who come from > 60 different institutes. International collaborations are also pursued actively, and the number of visiting foreign researchers reaches ~70. 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

UVSOR has several angle-resolved photoemission spectroscopy (ARPES) beamlines and users can choose proper beamline according to their purpose. At BL7U, users can perform high-energy resolution measurements with extremely low energy of photons (6 eV~) using low-temperature 6-axis manipulator with sample temperature 4 K.

For a long time, when changing photon energies in this beamline, users themselves had to optimize the beamline by using motors to adjust the mirror angle of the beamline to maximize the photon flux at the endstation. This was due to the lack of reproducibility of the position and angle of the mirrors by the motors. Recently, we performed ray-trace simulations and found that the mirror angle at which the photon flux is maximized is optically using the edge of the diffraction grating, which does not yield the correct photon energy. In fact, for some users, there was a difference of up to 500 meV between the actual photon energy and the set photon energy. This was a major problem for a high-energy-resolution beamline discussing a 1 meV superconducting gap, and made it difficult to perform automatic photon energy dependent ARPES measurements.

Therefore, we reviewed the mechanics of mirror position and angle control and introduced new motor control settings accordingly, and succeeded in precise control of photon energy with excellent reproducibility. As a result, we succeeded in setting the optically correct mirror angle, which enabled us to provide users with the correct photon energy within ±3 meV over the entire photon energy range available at BL7U ($h\nu$ = 6–40 eV). Users no longer need to adjust the mirror angle themselves. It should be noted that while many synchrotron radiation facilities have problems with photon energy reproducibility and energy drift with time at the endstations due to cooling problems of mirrors and changes in the electron trajectory of the accelerator and so on, BL7U is a normal-incident beamline, which is less susceptible to these problems. This is another reason why we were able to control photon energy so precisely. Having achieved accurate photon energy control, we plan to introduce various automated ARPES measurements in the future, including automatic photon energy dependent measurements.

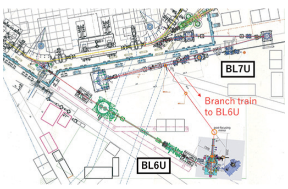


Figure 1. Schematic view of beamlines BL7U and BL6U. The low-energy photon of BL7U will be introduced to BL6U for multi-modal experiments.

Research Highlights

We started to develop resonant soft X-ray scattering (RSoXS) at BL3U. RSoXS can be used similarly to small angle X-ray scattering (SAXS) and can provide information on samples' mesoscopic structure (1 ~ 100 nm). Due to the resonance process, RSoXS have selectivities of elements, functional groups, and molecular orientations. In particular, since SX regions include K-edge energies of light elements such as carbon, nitrogen, and oxygen, RSoXS will be a powerful tool to investigate soft matter such as liquid-crystal and polymer materials, mainly consisting of light element atoms. Wang group in ALS recently applied the carbon K-edge RSoXS method to investigate polymer blends, block copolymers, organic bulk heterojunction solar cells, and polymeric transistors, as all of which the complex refractive indices of the different components have distinct energy and polarization dependences for X-ray energies near the edge.

As a first experiment, RSoXS was applied to the helical filamentary phase of liquid-crystals, a twist-bend liquid-crystal phase. As shown in Figure 2(a), the structure has spatial periodicity without electron density modulation. The sample is sandwiched with SiN and isolated from the vacuum. In addition, the sample temperature was controlled from 0 to 150 °C, and the structure was analyzed in various phases.

Figure 2(b) shows typical scattering RSoXS images at carbon K edge for helical nanofilaments.[1)] Photon energies were 285 and 270 eV, corresponding to carbon K-edge resonance and non-resonance energies. Diffraction rings derived from a clear periodic structure were observed at the resonant energy. For the resonant RSoXS image, the scattering angle 2θ is approximately 3°, corresponding to 80 nm. This pitch corresponds to the half pitch of the helical structure. Conventional SAXS cannot unravel helical structures due to no electron density modulation. Thus, by observing the molecular orientation order, we succeeded in characterizing the helix pitch of self-assembled liquid-crystal materials in situ.

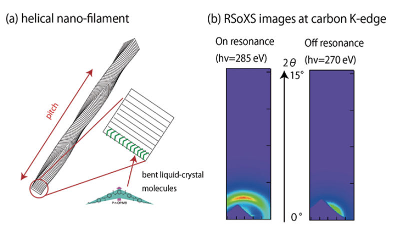


Figure 2. (a)Self assembled helical nanofilament of bent liquid-crystal molecules. (b) RSoXS images of helical nanofilaments at photon energies of 285 eV (resonance) and 270 eV (non-resonance).

Reference

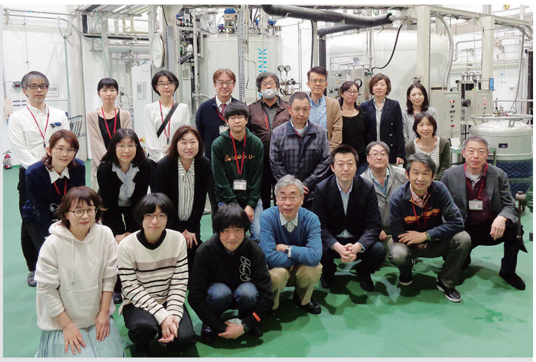
1) Y. Takanishi *et al.*, *RSC Adv.* **12**, 29346 (2022).

Award

NAKAMURA, Eiken; The 10th Japan Society for Synchrotron Radiation Research (JSSRR) Achievement Award (2023).

Instrument Center

YOKOYAMA, Toshihiko	Director, Professor
SUZUKI, Toshiyasu	Team Leader
NAKAMURA, Toshikazu	Team Leader
MINATO, Taketoshi	Senior Researcher
SHIGEMASA, Eiji	Unit Leader
TAKAYAMA, Takashi	Chief Engineer
FUJIWARA, Motoyasu	Chief Technician
UEDA, Tadashi	Chief Technician
ASADA, Mizue	Chief Technician
OKANO, Yoshinori	Technician
URUICHI, Mikio	Technician
MIYAJIMA, Mizuki	Technician
NAGAO, Haruyo	Technician
HIRANO, Kaho	Technician
ISHIYAMA, Osamu	Project Manager
NAKAMOTO, Keiichi	Project Manager
OTA, Yasuhito	Project Manager
KAKU, Mie	Project Manager
OHARA, Mika	Research Fellow
IKI, Shinako	Technical Fellow
FUJIKAWA, Kiyoe	Technical Fellow
KUBOTA, Akiko	Technical Fellow
IMAI, Yumiko	Technical Fellow
FUNAKI, Yumiko	Secretary
HYODO, Yumiko	Secretary
ISHIKAWA, Azusa	Secretary
UCHIDA, Mariko	Secretary
KURITA, Yoshiko	Secretary
TOYAMA, Yu	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 measurement apparatuses, 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 repaired in 2022–2023 and JNM-ECZL 600 installed in 2023 for solutions, and JNM-ECS400 for solutions), matrix assisted laser desorption/ionization time-of-flight (MALDI TOF) mass spectrometer (microflex LRF, Bruker Daltonics), ESI-TOF mass spectrometer (Bruker Daltonics, maXis), powder X-ray diffractometer (Rigaku RINT-Ultima III), molecular structure analysis using crystalline sponge method (Rigaku SuperNova), circular dichroism (CD) spectrometer (JASCO J-1500), differential scanning calorimeter (MicroCal VP-DSC), isothermal titration calorimeter (MicroCal PEAQ-iTC & iTC200), scanning electron microscope (SEM; JEOL JSM-6700F), elemental analyzer (J-Science Lab Micro Corder JM10), and ICP atomic emission spectroscopy (Agilent 5110 ICP-OES).

In the Myodaiji campus, the following instruments are installed: Electron spin resonance (ESR) spectrometers (Bruker E580 installed in 2022, E680, E500, EMX Plus, ns pulsed laser for time resolved experiments), NMR spectrometer (Bruker AVANCE600 for solids), superconducting quantum interference devices (SQUID; Quantum Design MPMS-7, MPMS-XL7, and MPMS-3 installed in 2022), solid-state calorimeter (Rigaku DSC8231/TG-DTA8122), solution X-ray diffractometer (Rigaku NANO-Viewer), single crystal X-ray diffractometers (Rigaku Mercury CCD-1, CCD2, RAXIS IV, and Rigaku HyPix-AFC), operando multipurpose x-ray diffraction for powder and thin films (Panalytical Empyrean), thermal analysis instruments (Rigaku DSC8231/TG-DTA8122), fluorescence spectrometer (SPEX Fluorolog), UV-VIS-NIR spectrometer (Shimadzu UV-3600Plus), Absolute PL quantum yield measurement (Hamamatsu Photonics Quantaurus-QY C11347-01), Raman microscope (Renishaw INVIA REFLEX 532), picosecond tunable laser system (Spectra Physics Tsunami and Quantronix Titan/Light Conversion TOPAS), low vacuum analytical SEM (Hitachi SU6600), field emission transmission electron microscope (JEOL JEM-2100F), angle resolved ultraviolet photoelectron spectroscopy (ARUPS) for functional band structures (Scienta-Omicron DA30), FTIR spectrometer (Bruker IFS 66v/S), two sets of *operando* scanning probe microscopes (Bruker Dimension XR Icon Nanoelectrical & Nanoelectrochemical), and electron spectrometers for chemical analysis (ESCA) equipment (Scienta-Omicron, R4000L1).

In the fiscal year of 2022, Instrument Center accepted 101 applications from outside and the total user time amounted 1,615 days for outside and 1,276 days for in-house. Instrument Center also maintains helium liquefiers in the both campus and provides liquid helium to users (51,198 L/year). Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute (41,816 L/year).

Instrument Center also organizes the Inter-University Network for Common Utilization of Research Equipments, the Molecule and Material Synthesis Platform in the Nanotechnology Platform Program (FY2012–2021), and the ARIM (Advanced Research Infrastructure for Materials and Nanotechnology in Japan) Program (FY2021–2030) 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
KONDO, Takuhiko	Chief Engineer (Unit Leader)
TOYODA, Tomonori	Chief Engineer
MATSUO, Junichi	Chief Technician
TAKADA, Noriko	Chief Technician
KIMURA, Sachiyo	Technician
KIKUCHI, Takuro	Technician
KIMURA, Kazunori	Technician
MIYAZAKI, Yoshino	Technician
SAWADA, Toshihiro	Technical Fellow
ISHIKAWA, Akiko	Technical Fellow
MIZUTANI, Nobuo	Technical Fellow
SUGANUMA, Kouji	Technical Fellow
INAGAKI, Itsuko	Secretary

Research and development 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, mechatronics, electronics and lithography 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 12-bit A/D Conversion Module with Contact Output

It would be useful to have a module that monitors the input analog voltage and reacts when the input voltage exceeds a threshold value. For example, it could be used to monitor abnormalities in the output voltage of laboratory equipment. For such purpose, it is enough to work in the low frequency range input of DC ~ a few kHz. We have developed such a module with a very simple configuration (Figure 1).

The input voltage range is from 0 to 5 V and threshold voltage can be adjusted using variable resistors. If the input voltage crosses the threshold, the contact output is shorted. A comparator (LM2903M by Texas Instruments) with hysteresis characteristics is provided in the front stage of the contact output to suppress the unexpected output due to slight fluctuations in input voltage near the threshold. Insulated BNC receptacle connector is used for both input and output. It works standalone by supplying 9V from the DC jack. It is also equipped with a Pmod interface for SPI communication. This interface can be used to supply power as well as to communicate with the built-in 12-bit A/D converter (MCP3221 by Microchip Technology) that can provide read input voltage values. In addition, despite the small size (45×90×25 mm) of the housing, the distance between the input and output BNC connectors is designed so as not to interfere with cable insertion and removal.

Figure 1. Module overview.

Molecular Modeling with Transparent Materials

We accept requests for making models of molecules and proteins. Scientists use these models to imagine their responses and behaviors in nanoscale. Models are also used to explain the research results in a lucid way.

3D printers are indispensable for making models. Since we introduced a full-color plastic 3D printer 3DUJ-2207 (Mimaki Engineering, Nagano, Japan) last year, we are now able to provide models with transparent resins. By using this, we can embed a full-color ribbon model in a transparent surface model (Figure 2), for example. When the ribbon model is placed in water, transparency of the ribbon model increases (Figure 3). In addition, we have made crystal models with transparent or semi-transparent crystal facets (Figure 4).

We would like to continue to contribute to the research activities of the Institute for Molecular Science by upgrading our technologies and skills.

Figure 2. Clear surface & ribbon model.

Figure 3. Underwater visibility of a model shown in Figure 2.

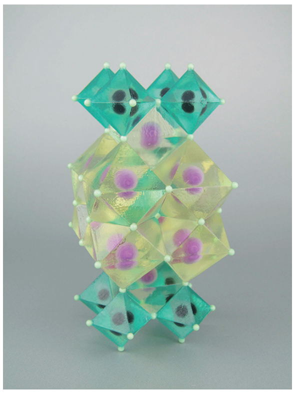


Figure 4. Crystal model with crystal facets.

Research Center for Computational Science (Okazaki Research Facilities)

EHARA, Masahiro	Director, Professor
SAITO, Shinji	Professor
OKUMURA, Hisashi	Associate Professor
OKAZAKI, Kei-ichi	Associate Professor
OONO, Hitoshi	Associate Professor
UCHIYAMA, Ikuo	Associate Professor
OHNUKI, Jun	Assistant Professor
SHIRAOGAWA, Takafumi	Assistant Professor
ISHIDA, Tateki	Research Associate
IWAHASHI, Kensuke	Chief Engineer (Unit Leader)
MIZUTANI, Fumiyasu	Engineer
NAITO, Shigeki	Chief Technician
KAMIYA, Motoshi	Chief Technician
SAWA, Masataka	Technician
NAGAYA, Takakazu	Technician
KINOSHITA, Takamasa	Technician
SUZUKI, Kazuma	Technician
KANESHIRO, Ikuma	Technician
YAZAKI, Toshiko	Technical Fellow
UNO, Akiko	Technical Fellow
KONDO, Noriko	Secretary
URANO, Hiroko	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, basic biology, and physiology. Our systems consist of HPE Apollo 2000 and Apollo 6500 (since Feb. 2023). The combined system, named "Molecular Simulator," is ranked 196th position in the TOP500 supercomputer list in June 2023. 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 about 30 application programs to the users: Gaussian, GAMESS, Molpro, AMBER, Gromacs, and so on. In particular, we have implemented some original programs developed by researchers in Japan to provide them to the users. The supercomputer systems had been used by 1,242 researchers from 298 groups in fiscal year 2022. Some of the computational resources are provided to the following projects: Program for Promoting Research on the Supercomputer Fugaku, Professional development Consortium for Computational Materials Scientists (PCoMS), and Elementary Strategy Initiative to Form a Core Research Center.

For fostering young generation, we organize the schools of quantum chemistry and molecular dynamics simulation every year. In the fiscal year 2022, the numbers of registered attendants of these schools were 360 and 414, respectively. We also organize the RCCS supercomputer workshop focusing on the new trends of computational chemistry for the purpose of the research exchange and human resource development. In the fiscal year 2022, we organized the workshop under the title, "Theoretical and Computational Science for Complex Electronic States."

In cooperation with Institute for Materials Research, Tohoku University, Institute for Solid State Physics, University of Tokyo, and Nanoscience Design Center, Osaka University, we established the Computational Materials Science Forum (CMSF) to promote the cutting-edge computational materials science technology of Japan, to create world-class results, and to realize the social implementation of simulation technology and materials information science technology.

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. 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. 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/).

The center is jointly managed with National Institute for Physiological Sciences and National Institute for Basic Biology (both in the same campus).

Figure 1. HPE Apollo 2000 and Apollo 6500.

Safety Office

TANAKA, Shoji	Director
TOMURA, Masaaki	Research Associate
SHIGEMASA, Eiji	Technical Associate
UEDA, Tadashi	Technical Associate
TAKAYAMA, Takashi	Technical Associate
SAKAI, Masahiro	Technical Associate
MAKITA, Seiji	Technical Associate
MATSUO, Junichi	Technical Associate
KIKUCHI, Takuro	Technical Associate
TSURUTA, Yumiko	Secretary
ASAKURA, Yukiko	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.