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 (1978–2018).

UVSOR Synchrotron Facility

KERA, Satoshi	Director, Professor
KATOH, Masahiro	Project Professor
TANAKA, Kiyohisa	Associate Professor
MATSUI, Fumihiko	Senior Researcher
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OHIGASHI, Takuji	Assistant Professor
IDETA, Shin-ichiro	Assistant Professor
FUJIMOTO, Masaki	Assistant Professor
MATSUDA, Hiroyuki	Post-Doctoral Fellow
NAKAMURA, Eiken	Technical Assosiate
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
YUZAWA, Hayato	Technical Associate
HORIGOME, Toshio	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 undulators are in- vacuum soft X-ray (SX) linear-polarized undulators

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.

(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. 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. Since 2018, BL1U is partly opened for using as 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.

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 11 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

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.

An acceptance-cone-tunable (ACT) electron spectrometer for the highly-efficient constant-energy photoelectron mapping of functional materials was developed at BL6U. The ACT spectrometer consists of the concentric hemispherical analyzer with the mesh-type electrostatic lens near the sample. The acceptance cone of the spectrometer is expanded by a factor of up to 3.3 by applying a negative bias to the sample and grounding the mesh lens and the analyzer entrance. The wide-angle observation of the valence band dispersion over full Brillouin zone can be easily achieved without rotating / tilting the sample nor analyzer.

The UVSOR accelerators have been operated for more than 35 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)]

X-ray microscopy has the following advantages for the observation of biological samples over other microscopic methods: Higher resolution than optical microscopy with respect to the diffraction limit; good absorption contrast in hydrated conditions with soft X-rays in an energy range, the so-called water window; better transmittance than electron microscopy; and the discrimination of biological molecules by spectromicroscopy, the combination of microscopy and spectroscopy using absorption of fine structures in biomolecules according to the energies of carbon, nitrogen, and oxygen absorption edges. Scanning transmission soft X-ray microscopy (STXM) was applied to study the quantitative distribution of DNA, RNA, histone, and proteins other than histone (represented by BSA) in mammalian cells, apoptotic nuclei, and a chromosome at BL4U. Quantities of nucleic acids and proteins were evaluated using characteristic absorption properties due to the 1s–π^* transition of N=C in nucleic acids and amide in proteins, respectively, in the absorption spectra at the nitrogen K absorption edge. The results showed that DNA and histone were located in the nucleus. By contrast, RNA was clearly discriminated and found mainly in the cytoplasm. Interestingly, in a chromosome image, DNA and histone were found in the center, surrounded by RNA and proteins other than histone. The amount of DNA in the chromosome was estimated to be 0.73 pg, and the content of RNA, histone, and proteins other than histone, relative to DNA, was 0.48, 0.28, and 4.04, respectively. STXM could be a powerful approach for the quantitative molecular mapping of biological samples at high resolution.

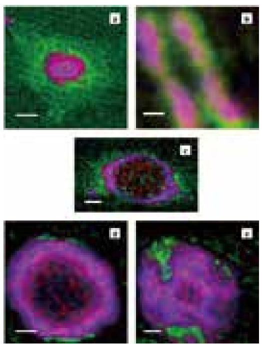

Figure 2. RGB expression of the images of the (a) CHO cell, (b) chromosome, (c) HeLa S3 cell, (d) isolated nucleus, and (e) apoptotic nucleus. DNA, RNA, and histone are displayed as red, green, and blue, respectively. Scale bars are (a) 5 µm, (b) 0.5 µm, (c) 2 µm, and (d, e) 1 µm.

Reference

1) K. Shinohara *et al.*, *Cells* **8**, 164 (2019).

Center for Mesoscopic Sciences

OKAMOTO, Hiromi	Director, Professor
OHMORI, Kenji	Professor
IINO, Ryota	Professor
TAIRA, Takunori	Associate Professor
FUJI, Takao	Associate Professor
SUGIMOTO, Toshiki	Associate Professor
NARUSHIMA, Tetsuya	Assistant Professor
YOSHIZAWA, Daichi	Assistant Professor
ISHIZUKI, Hideki	Assistant Professor
NOMURA, Yutaka	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.

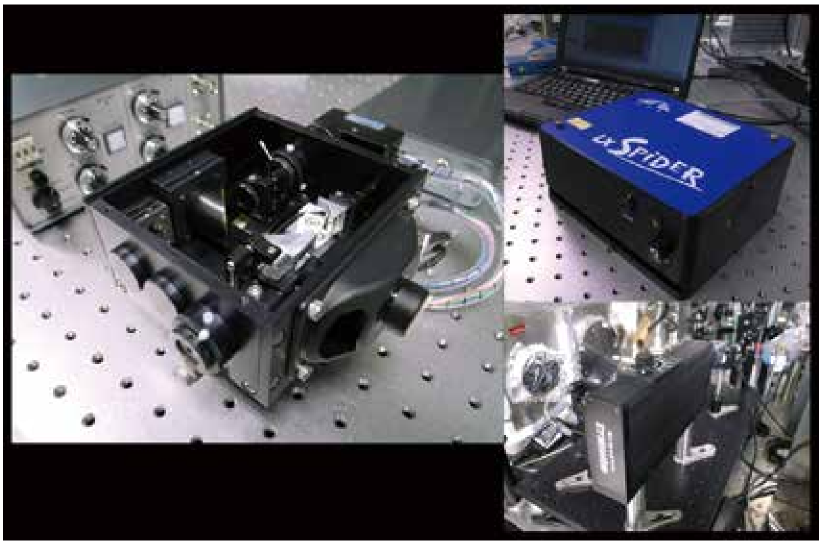

Figure 1. (left) A Fringe-Resolved Autocorrelation (FRAC) apparatus for sub-10 fs pulse characterization designed in the Center. (upper right) Spectral Phase Interferometry for Direct Electric-Field Reconstruction (SPIDER) and (lower right) Frequency-Resolved Optical Gating (FROG) apparatuses for general-purpose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

Instrument Center

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NAKAMURA, Toshikazu	Team Leader
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FUJIWARA, Motoyasu	Technical Associate
OKANO, Yoshinori	Technical Associate
MIZUKAWA, Tetsunori	Technical Associate
UEDA, Tadashi	Technical Associate
ASADA, Mizue	Technical Associate
OHARA, Mika	Project Manager
HIGASHI, Yosuke	Project Manager
ISHIYAMA, Osamu	Project Manager
HASEGAWA, Hisashi	Project Manager
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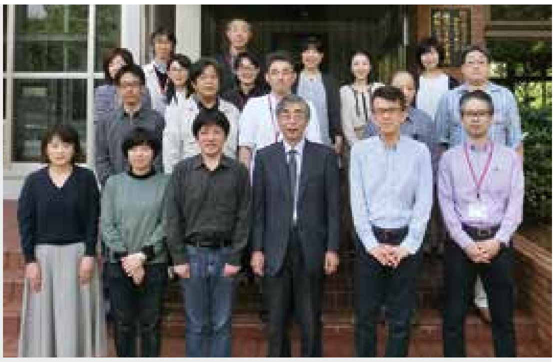
IKI, Shinako	Technical Fellow
NAGAO, Haruyo	Technical Fellow
MATSUO, Yukiko	Technical Fellow
FUJIKAWA, Kiyoe	Technical Fellow
YOKOTA, Mitsuyo	Secretary
FUNAKI, Yumiko	Secretary
HYODO, Yumiko	Secretary
TOYAMA, Yu	Secretary
IWANO, Yukie	Secretary
SHIBATA, Yuka	Secretary
ISHIKAWA, Azusa	Secretary
KATO, Kaori	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) 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, ns pulsed laser for time resolved experiments), 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 Rigaku HyPix-AFC), molecular structure analysis using crystalline sponge method (Rigaku XtaLAB P200/PILATUS 200K, Rigaku SuperNova), thermal analysis instruments (Rigaku DSC8231/TG-DTA8122), fluorescence spectrometer (SPEX Fluorolog2), X-ray fluorescence spectrometer (JEOL JSX-3400RII), UV-VIS-NIR spectrometer (Shimadzu UV-3600Plus), Raman microscope (Renishaw INVIA REFLEX 532), 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 2018, new equipment of high-performance thin film and powder x-ray diffractometer and atomic force microscopes will be installed. Instrument Center accepted 102 applications from outside and the total user time amounted 2,424 days for outside and 610 days for in-house with 29 equipments. Instrument Center also maintains helium liquefiers in the both campus and provides liquid helium to users (45,606 L/year). Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute (38,768 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.

Award

TAKAYAMA, Takashi; The Chemical Society of Japan Award for Technical Achievements for 2018.

Equipment Development Center

YAMAMOTO, Hiroshi	Director
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AOYAMA, Masaki	Technical Associate
KONDOU, Takuhiko	Technical Associate
TOYODA, Tomonori	Technical Associate
TAKADA, Noriko	Technical Associate
KIMURA, Sachiyo	Technical Associate
KIKUCHI, Takuro	Technical Associate
KIMURA, Kazunori	Technical Associate
SAWADA, Toshihiro	Technical Fellow
YOSHIDA, Hisashi	Technical Fellow
ISHIKAWA, Akiko	Technical Fellow
URANO, Hiroko	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 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.

Introduction of Electroplating Technology

In the Equipment Development Center (EDC), precise metal patterns are made by spattering after lithography. However, it is difficult to deposit those metals with the thickness more than 10 micrometers that is needed to produce self-standing items like a metal mask or beam stop. In order to achieve those required thicknesses, we are considering the introduction of plating technology.

As a first example, we tried to produce a molecular beam skimmer by electroforming: EDC has an experience of producing a skimmer by machining. However, it was difficult to fabricate a skimmer whose thickness is less than 1mm or to fabricate one with a small hole on the tip because of technical limitation. With electroforming, one can expect a thin metal structure which has been impossible by machining.

For this purpose, we started the process by making a lab size plating equipment and by selecting nickel sulfamate as electrolyte which is often used for electroforming. The electrodeposition by this electrolyte is advantageous in preventing deformation after plating because of smaller stress than those from other reagents. The skimmer was produced after two and half hours, whose deposit thickness was about 100 micrometers. (Figure 1) We also tested outsourced products, but they were difficult to release from the mold. On the other hand, our product was able to be released to give the skimmer easily because of the optimized pretreatment conditions by ourselves. By utilizing the difference in thermal expansion coefficient of materials, the release of the skimmer from the mold was performed by temperature cycling.

In the near future, we will study and manufacture the optimal shape of the mother mold and aim to incorporate it into the actual experimental equipment for molecular science.

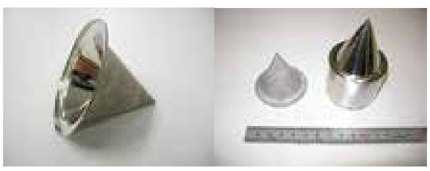


Figure 1. Molecular beam skimmer made by Electroforming.

Signal Fan-Out Buffer and Distributor

In experiments using a pulsed laser such as time-dependent spectroscopy on a reaction process, a delayed pulse generator which provides signals with both a long delay time T_d and a short time-width T_w that are triggered by the laser pulse is required. When the size of the target molecule is large, T_d is increased to several milliseconds or longer. On the other hand, in order to collect only the necessary part of reaction signals into a measurement system, T_w should be as short as several microseconds.

We have developed a Delayed Pulse Generator (Figure 2) which satisfies the above specification using an ARM microcontroller (NXP LPC1114FBD48/302) and FPGA (Xilinx XC7A35T-1CPG236C) microchip. The time resolution of this equipment is 5 ns both in T_d and T_w, while the setting range of T_d is 0 ns to 4 sec, and the setting range of T_w is 1 µs to 100 ms. In addition, this equipment has a monitor output for trigger signals, with an output impedance of 50 ohms which is the same as that for output pulse.

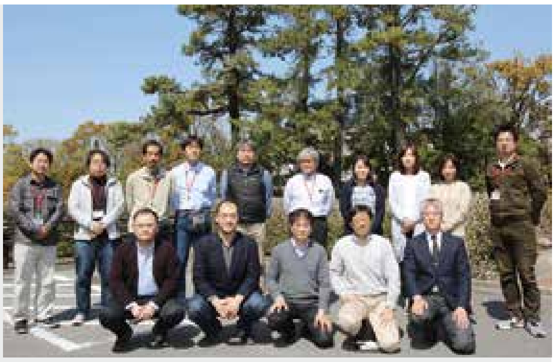
Figure 2. Inside of a Delayed Pulse Generator (1ch version).

Award

MIZUTANI, Nobuo; The Chemical Society of Japan Award for Technical Achievements for 2018.

Research Center for Computational Science

EHARA, Masahiro	Director, Professor
SAITO, Shinji	Professor
OKUMURA, Hisashi	Associate Professor
OONO, Hitoshi	Assistant Professor
ISHIDA, Tateki	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	Technical Associate
UNO, Akiko	Technical Fellow
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 (until Sep. 2018). The NEC LX 406Rh-2 and 110-Rh1 combined system, named "Molecular Simulator," is ranked 153rd position in the TOP500 supercomputer list in June 2019. 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 913 researchers from 237 groups in fiscal year 2018. 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

TANAKA, Shoji	Director
TOMURA, Masaaki	Research Assistant
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.