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
KATOH, Masahiro	Project Professor
TANAKA, Kiyohisa	Associate Professor
TAIRA, Yoshitaka	Associate Professor
MATSUI, Fumihiko	Senior Researcher
IWAYAMA, Hiroshi	Assistant Professor
OHIGASHI, Takuji	Assistant Professor
IDETA, Shin-ichiro	Assistant Professor
FUJIMOTO, Masaki	Assistant Professor
SUGITA, Kento	Assistant Professor
MATSUDA, Hiroyuki	Post-Doctoral Fellow
SALEHI, Elham	Post-Doctoral Fellow
HAYASHI, Kenji	Engineer (Unit Leader)
NAKAMURA, Eiken	Chief Engineer
MAKITA,Seiji	Engineer
YAMAZAKI, Jun-ichiro	Chief Technician
SAKAI, Masahiro	Chief Technician
YANO, Takayuki	Chief Technician
OKANO, Yasuaki	Chief Technician
TESHIMA, Fumitsuna	Technician
KONDO, Naonori	Technician
YUZAWA, Hayato	Technician
OTA, Hiroshi	Technician
HORIGOME, Toshio	Technical Fellow
MINAKUCHI, Aki	Technical Fellow
MIZUKAWA, Tetsunori	Technical Fellow
ISHIHARA, Mayumi	Secretary
KAMO, Kyoko	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. The BL1U can produce pulsed γ-ray radiation by laser Compton scattering technique. In 2021, it was developed by constructing a laser transport system to generate high-intense γ-ray beams. 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 > 4000, 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. COVID-19 issue has a serious impact on user activity, the overseas activity was almost dropped especially. The fruits of the research activities using UVSOR-III Synchrotron are published as the UVSOR ACTIVITY REPORT annually.

Recent Developments

The UVSOR accelerators have been operated for 38 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.

On the other hand, we are also putting effort into setting up state-of-the-art experimental stations that takes advantage of our unique beamline performance. BL5U is an angle-resolved photoemission spectroscopy (ARPES) beamline with micro-focused beam (23×40 µm). By combining the latest version of ARPES analyzer (MB Scientific AB, A-1 analyzer Lens#5) with the super quick deflector scan mode, users can perform ARPES measurements on small samples or inhomogeneous samples without changing the sample position. In 2020, a new spin-resolved ARPES system with multi-channel detection (we call "image-spin" detection) has been installed. As shown in Figure 1, we successfully obtained spin-resolved ARPES image of Rashba spin splitting in Au(111) surface states, which was taken at once. According to the rough estimation, the efficiency is 100 times better and the momentum resolution is several times better than the current synchrotron-based ARPES with single-channel detection in the world.

UVSOR has several ARPES beamlines and users can choose proper beamline according to their purpose. At BL7U, high-energy resolution ARPES is available with extremely low energy of photons (6 eV~) using low-temperature 6-axis manipulator (4 K~). In BL6U, photoelectron momentum microscope (PMM), which is an electronic spectroscopy with both the real space and momentum space resolution, has been installed in February 2020 (SPECS Surface Nano Analysis GmbH, KREIOS 150 MM).[1] It will be upgraded to a double hemispherical analyzer in FY2021 and will have spin-resolved function in the future.

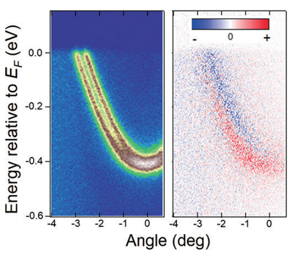

Figure 1. Rashba spin splitting in Au(111) surface states (left) and spin-resolved ARPES image showing the spin polarization (right).

Reserch Highlights

One of the highlights of the UVSOR research activities this year is the discovery of an ultrathin liquid cell for X-ray absorption spectroscopy (XAS) in the low-energy region at BL3U. Recently, we have investigated local structures of several aqueous solutions and various chemical processes in solution such as catalytic and electrochemical reactions and laminar flows in microfluidics by using *operando* XAS in C, N, and O K-edges.[2,3] On the other hand, the low-energy region below 200 eV is important for chemical research since it includes K-edges of Li and B and L-edges of Si, P, S, and Cl. BL3U has an advantage to measure XAS in the low-energy region with a high photon flux. Recently, we have established an argon gas window that is effective from 60 to 240 eV with the removal of high order X-rays.[4] The SX transmission calculation proposed that XAS in the low-energy region needs an ultrathin liquid cell with the 2.6 mm optical length of Ar gas.

Figure 2 shows the XAS measurement system including the ultrathin liquid cell. The ultrathin liquid cell is in an atmospheric Ar condition and is separated from the beamline and a photodiode detector under ultrahigh vacuum conditions with Si_3N_4 membranes (0.2 × 0.2 mm^2). The 2.6 mm optical length of argon gas has been realized owing to the ultrathin liquid cell. XAS spectra of 2 M LiCl solutions at Li K-edge and Cl L-edge were successfully obtained by using this liquid cell. In the future, XAS in the low-energy region will be applied to various chemical processes in solution, such as a Li-ion battery, Ni-borate electrocatalysts, and organic reactions with organosilicons, organolithiums, and organoboranes.

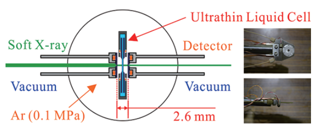

Figure 2. A schematic of the XAS measurement system in the low-energy region including the ultrathin liquid cell. Photographs of the ultrathin liquid cell are also shown.

References

1) F. Matsui *et al.*, *Jpn. J. Appl. Phys.* **59**, 067001 (2020).

2) M. Nagasaka *et al.*, *Anal. Sci.* **36**, 95 (2020).

3) M. Nagasaka and N. Kosugi, *Chem. Lett.* **50**, 956 (2021).

4) M. Nagasaka, *J. Synchrotron Radiat.* **27**, 959 (2020).

Awards

NAKAMURA, Eiken; The Chemical Society of Japan Award for Technical Achievements for 2020 (2021).

NAKAMURA, Eiken; The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology Outstanding Support for Research Award (2021).

Instrument Center

YOKOYAMA, Toshihiko	Director, Professor
SUZUKI, Toshiyasu	Team Leader
NAKAMURA, Toshikazu	Team Leader
MINATO, Taketoshi	Senior Researcher
MAKITA, Seiji	Engineer
TAKAYAMA, Takashi	Engineer
FUJIWARA, Motoyasu	Chief Technician
OKANO, Yoshinori	Technician
MIZUKAWA, Tetsunori	Technician
UEDA, Tadashi	Technician
ASADA, Mizue	Technician
URUICHI, Mikio	Technician
MIYAJIMA, Mizuki	Technician
OHARA, Mika	Project Manager
ISHIYAMA, Osamu	Project Manager
HASEGAWA, Hisashi	Project Manager
NAKAMOTO, Keiichi	Project Manager
IKI, Shinako	Technical Fellow
NAGAO, Haruyo	Technical Fellow
FUJIKAWA, Kiyoe	Technical Fellow
TOYAMA, Aya	Technical Fellow
FUNAKI, Yumiko	Secretary
HYODO, Yumiko	Secretary
TOYAMA, Yu	Secretary
ISHIKAWA, Azusa	Secretary
UCHIDA, Mariko	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), operando multipurpose x-ray diffraction for powder and thin films (Panalytical Empyrean), thermal analysis instruments (Rigaku DSC8231/TG-DTA8122), fluorescence spectrometer (SPEX Fluorolog), 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), angle resolved ultraviolet photoelectron spectroscopy (ARUPS) for functional band structures (VG-Scienta DA30), and FTIR spectrometer (Bruker IFS 66v/S). Recently, new equipment of high-performance *operando* scanning probe microscopes (Bruker Dimension XR Icon Nanoelectrical and Nanoelectrochemical, two sets) was just installed, and electron spectrometers for chemical analysis (ESCA) equipment (Scienta, R4000L1) was newly registered for public usage in Instrument Center. In the fiscal year of 2020, Instrument Center accepted 85 applications from outside and the total user time amounted 1,871 days for outside and 2,056 days for in-house with 26 equipments. Instrument Center also maintains helium liquefiers in the both campus and provides liquid helium to users (43,818 L/year). Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute (30,455 L/year). Instrument Center also 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
KONDO, Takuhiko	Chief Engineer (Unit Leader)
TOYODA, Tomonori	Engineer
MATSUO, Junichi	Chief Technician
TAKADA, Noriko	Technician
KIMURA, Sachiyo	Technician
KIKUCHI, Takuro	Technician
KIMURA, Kazunori	Technician
SAWADA, Toshihiro	Technical Fellow
YOSHIDA, Hisashi	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, mechanics, 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.

PDMS Mixing Chamber for Soft X-Ray Absorption Spectroscopy

We have fabricated a microfluidic device with flow paths for solution mixing, which is used for soft X-ray absorption spectroscopy. This flow device is equipped with two inclined channel paths which guide liquids to a mixing chamber in addition to a channel for outcoming flow. Width and depth of the flow paths are both 50 μm, and the pattern seen from above is Y-shaped. The diameters of the channels are 0.2 mm, and the bottom of the device is made of SiN membrane. We have produced these flow paths by casting PDMS (polydimethylsiloxane) into a mold. We have made the inclined channel paths by embedding three piano wires with a diameter of 0.2 mm before curing PDMS moiety (Figure 1). We have fixed these wires by using a guide produced by 3D printer. Since some issues have been found in the experiment, we are planning to improve this device.

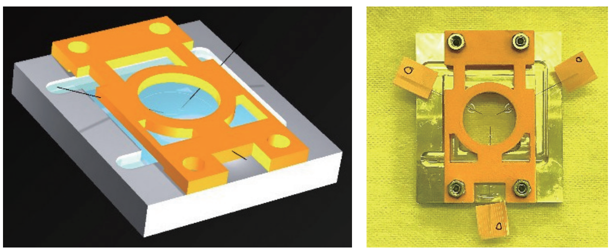

Figure 1. A 3D drawing (left) and picture (right) of the PDMS sample holder in a mold.

Improvement of ECL Logic Circuit with CPLD and Development of an Analog Level Converter

We have developed “a multi-coincidence electronic circuit for time-resolved reaction microscopy of electron Compton scattering” in collaboration with Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, in 2007. The circuit consists of many devices for emitter coupled logic (ECL) to process multiple signals transmitted from position-sensitive-detectors (PSDs).

We have received a request to improve the circuit for higher performance in another experiment. It requires a circuit to accept 13 inputs to be processed into one output signal in Nuclear Instruments Module (NIM) level. Pulse duration of input signals should be stretched using a monostable multivibrator. The output signal is generated by several logical operations. To simplify implementation of such operations, we decided to use CPLD (Complex Programmable Logic Device; XC2C256-7TQ144C by Xilinx) with analog level transducer circuit (Figure 2). All of logical operations are putted into single CPLD and tested by simulation. Level converter circuit that we have developed can convert NIM level pulses into TTL level in a 10 nanoseconds duration time scale (and vice versa) as we expected. We are planning to test them with a virtual system that reproduces the real experimental setup.

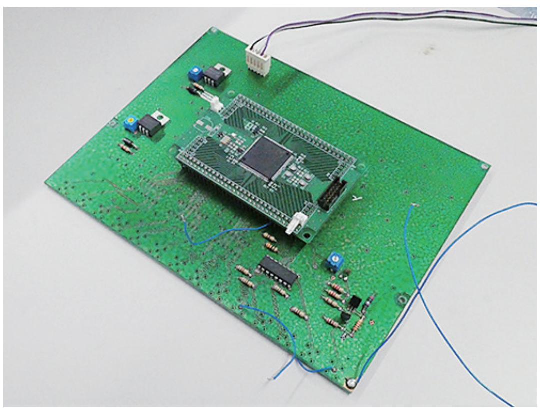

Figure 2. Level conversion circuit and CPLD board assembled for the performance evaluation.

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
ISHIDA, Tateki	Assistant Professor
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
YAZAKI, Toshiko	Technical Fellow
UNO, Akiko	Technical Fellow
KONDO, Naoko	Secretary
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, and physiology. Our systems consist of NEC LX (406Rh-2, 110-Rh1, 108Th-4G; since Oct. 2017). The NEC LX 406Rh-2 and 110-Rh1 combined system, named "Molecular Simulator," is ranked 261st position in the TOP500 supercomputer list in June 2020. 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 1,142 researchers from 271 groups in fiscal year 2020. 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. 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.

We organized a joint Supercomputer workshop of the Research Center for Computational Science and the Nanotechnology Platform Project, "Toward Collaboration between Theoretical/Computational Science and Experimental Science Based on Data Science" and two schools "The 10th Quantum Chemistry School" and "The 14th Molecular Simulation School—From Basics to Applications. 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 Council for Computational Materials Science 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. NEC LX.

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
TESHIMA, Fumitsuna	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.