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
TANAKA, Kiyohisa	Associate Professor
TAIRA, Yoshitaka	Associate Professor
OHIGASHI, Takuji	Associate Professor (Cross Appt.)
KANEYASU, Tatsuo	Associate Professor (SAGA-LS)
IWAYAMA, Hiroshi	Assistant Professor
SUGITA, Kento	Assistant Professor
FUJIMOTO, Masaki	Assistant Professor (Nagoya Univ.)
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
SUGIMOTO, Yasunobu	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 2022, 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 39 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.

UVSOR has several ARPES undulator beamlines and users can choose proper beamline according to their purpose. We are putting effort into setting up state-of-the-art experimental stations that take 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 ARPES analyzer with the super quick deflector scan mode, users can perform ARPES measurements on small samples or inhomogeneous samples without changing the sample position. At BL7U, high-energy resolution ARPES is available with extremely low energy of photons (6 eV~) using low-temperature 6-axis manipulator with sample temperature 4 K. In 2021, the latest version of ARPES analyzer has been installed so that users can easily perform a quick Fermi surface mapping. In BL6U, "photoelectron momentum microscope (PMM)" has been installed in February 2020.[1,2] PMM is a new concept device based on photoelectron spectroscopy and photoelectron microscopy techniques to visualize electronic states in real and reciprocal lattice space in selected small regions. It was upgraded to a double hemispherical analyzer with spin filter and spin rotator in May 2022.

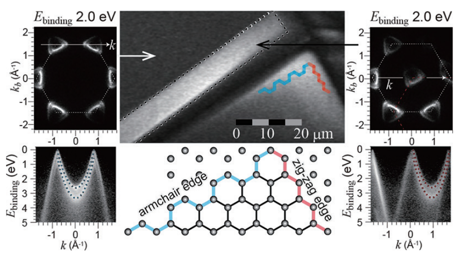

Figure 1. μm-photoelectron spectroscopy of graphite edge facet by PMM.

Reserch Highlights

At BL1U, new light sources such as coherent synchrotron radiation, free electron lasers, high-order harmonic generation, optical vortex and vector beams, and ultrashort pulsed gamma rays have been developed. As the energy of ultrashort pulsed gamma rays is 6.6 MeV, positrons are generated inside materials when they are irradiated. Positron annihilation spectroscopy is a powerful analytical tool for nondestructive measurement of atomic-scale defects. Positron annihilation spectroscopy using ultrashort pulsed gamma rays is available at BL1U.[3] In positron annihilation spectroscopy, the annihilation gamma rays produced when a positron annihilates are measured numerous times to determine the positron lifetime and the energy spread of the positron annihilation. Therefore, it is important to increase the counting rate of annihilation gamma rays in order to complete the measurement in a short time. To increase the counting rate of annihilation gamma rays, the intensity of ultrashort pulsed gamma rays should be increased. The intensity of gamma rays can be increased by colliding the electron beam and the laser in a focused state.

Until March 2021, gamma ray was generated using an optical window that allowed the laser to be injected from the vertical direction. The laser size at this time was 1 mm. The other side of the incident window is not a window but stainless steel, which generates gas when the laser hits it. The laser size could not be focused to a smaller size because of the problem of background bremsstrahlung gamma rays due to the increased gas generation when the laser is focused.

In April 2021, a new vacuum chamber for laser injection, shown in Figure 2, was installed in the electron storage ring. This vacuum chamber has optical windows at each end of the horizontal and vertical directions, which allows the laser to collide with the electron beam in a focused state. The intensity of the gamma rays can be improved as the laser can be injected from the horizontal direction. During installation of the vacuum chamber, 1/4 circumference of the electron storage ring was opened to the atmosphere.

The laser size at the electron beam interaction point with the new vacuum chamber is 15 μm at full width at half maximum. The gamma-ray intensity was increased by a factor of 40 due to the smaller laser size and the horizontal injection of the laser. Using this ultrashort pulse gamma-ray source, experiments such as analysis of atomic-scale defects in scintillators and photocatalysts, in-situ measurement of defect formation in iron-based materials under stress loading, and magnetic Compton scattering are underway.

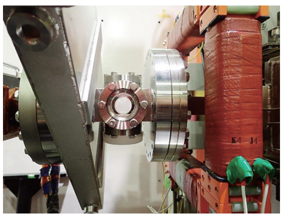

Figure 2. A new vacuum chamber for laser injection installed in the electron storage ring.

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2) F. Matsui *et al.*, *J. Phys. Soc. Jpn.* **91**, 094703 (2022).
3) M. Kitaura *et al.*, *Opt. Mater.: X* **14**, 100156 (2022).

Instrument Center

YOKOYAMA, Toshihiko	Director, Professor
SUZUKI, Toshiyasu	Team Leader
NAKAMURA, Toshikazu	Team Leader
MINATO, Taketoshi	Senior Researcher
TAKAYAMA, Takashi	Engineer
FUJIWARA, Motoyasu	Chief Technician
OKANO, Yoshinori	Technician
UEDA, Tadashi	Technician
ASADA, Mizue	Technician
URUICHI, Mikio	Technician
MIYAJIMA, Mizuki	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
NAGAO, Haruyo	Technical Fellow
FUJIKAWA, Kiyoe	Technical Fellow
TOYAMA, Aya	Technical Fellow
FUNAKI, Yumiko	Secretary
HYODO, Yumiko	Secretary
ISHIKAWA, Azusa	Secretary
UCHIDA, Mariko	Secretary
KURITA, Yoshiko	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 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), 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), solid-state calorimeter (Rigaku DSC8231/TG-DTA8122), scanning electron microscope (SEM; JEOL JSM-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 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 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), *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/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), and 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 2021, Instrument Center accepted 98 applications from outside and the total user time amounted 2,563 days for outside and 1,974 days for in-house with 31 equipments. Instrument Center also maintains helium liquefiers in the both campus and provides liquid helium to users (43,765 L/year). Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute (37,294 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	Engineer
MATSUO, Junichi	Chief Technician
TAKADA, Noriko	Technician
KIMURA, Sachiyo	Technician
KIKUCHI, Takuro	Technician
KIMURA, Kazunori	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, mechanics, electronics and lithography ones, 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.

Machining with High Accuracy

Researchers need new equipment to realize advanced experimental setups designed for their novel scientific achievements. We, the Equipment Development Center (EDC), receive various requests from researchers. For example, there is a plastic pipe shaped as shown in Figure1. This product was made by a precision lathe owned by the EDC shown in Figure 2, the process of which is full of ingenuity by the staffs with the knowledge on the materials properties. (Figure 3)

The pipe is designed to connect to a custom-made equipment as a gas tube adapter. A commercial product cannot be connected to the equipment due to a limitation in space. Furthermore, tolerance is very strict and needs to be less than 5/1000mm, because a high-pressure gas may blow the tube away from the equipment.

Such strict requirements are difficult to be handled by outsourcing. Even if it is possible, the cost is unreasonably high, or the product may not be available on schedule. We respond to such request from researchers with quick delivery, meticulous work, and less costs in order to contribute to their experiments which will lead to scientific advancements.

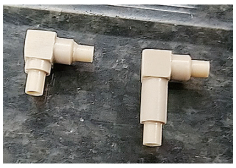

Figure 1. Plastic Pipe.

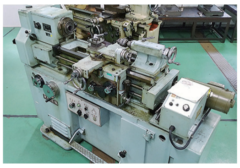

Figure 2. Precision Lathe.

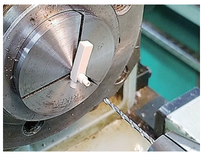

Figure 3. Machining a pipe.

Fabrication of a Signal Splitter

In order to synchronize an AFM system with lock-in amplifier, it is necessary to amplify the system signal whose frequency and amplitude are in the range from 200 kHz to 250 kHz and about 100 mVp-p, respectively, by about 10 times. In addition, when the input signal to the lock-in amplifier has jitter, synchronization cannot be achieved. Thus it is required to remove unnecessary frequency components and amplify the signal with high precision. It is also required to split the signal into two circuits before the amplification for the sake of simultaneous topographic observation. Moreover, an current output which can drive the 50Ω input impedance of the measurement system is mandatory.

We have developed a Signal Splitter shown in Figure 4; it buffers the signal detected by AFM with high input impedance by JFET type operational amplifier (Analog Devices AD825ARZ), and cuts unnecessary frequency components off by active high-pass filter with a cutoff frequency of 100 kHz. Then the signal is amplified by 6 times with another operational amplifier (Analog Devices AD8639ARZ), which allows driving of 50Ω impedance with the help of current feedback operational amplifier (Texas Instruments THS3001CD).

This instrument has enabled vibrational spectroscopy of single proteins and ultrafast nano-spectroscopy.

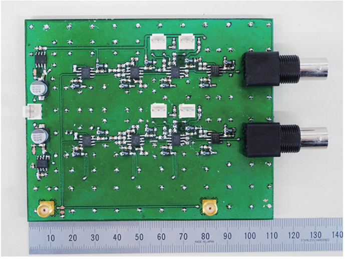

Figure 4. The Circuit Board of the Signal Splitter.

Award

TOYODA, Tomonori; The Chemical Society of Japan Award for Technical Achievements for 2021 (2022).

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
ISHIDA, Tateki	Research Assistant
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, 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 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 448th position in the TOP500 supercomputer list in June 2022. 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 1,175 researchers from 278 groups in fiscal year 2021. 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 2021, the numbers of registered attendants of these schools were 482 and 377, 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 2021, we organized the workshop under the title, "Computational science of structure, function and design of biomolecules."

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. 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
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.