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
MATSUDA, Hiroyuki	Post-Doctoral Fellow
SALEHI, Elham	Post-Doctoral Fellow
HAYASHI, Kenji	Technical Associate
NAKAMURA, Eiken	Technical Assosiate
YAMAZAKI, Jun-ichiro	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
OKANO, Yasuaki	Technical Associate
HORIGOME, Toshio	Specially Appointed Technical Associate
MINAKUCHI, Aki	Technical Fellow
INAGAKI, Itsuko	Secretary
ISHIHARA, Mayumi	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 53 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 (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.

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 number of visiting researchers per year tops > 1200, whose 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 proposals of 63 % have been achieved so far. 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 37 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. A new photoelectron momentum microscope (PMM) station for 3D momentum-resolved photoelectron spectroscopy is constructed at beamline BL6U.[1] The PMM, a combination of projection-type electron analyzer and photoelectron microscope, simultaneously realizes a microscope function for magnifying and observing minute parts of complicated- structured samples with element selectivity and a spectroscopy function for visualizing electron behavior (momentum) that determines the electronic properties of a functional materials. Microscopy with a spatial resolution of 50 nm and photoelectron spectroscopy (field of view: 2 μm) with energy/momentum resolutions of 20 meV / 0.01 Å^{-1} at 9 K are successfully demonstrated (Figure 1). The momentum microscope opens the door to direct observation of the Fermi surface and band structure of μm-sized targets such as surface atomic sites, thin films and interfaces, molecular adsorbates, and polycrystals, which was difficult with conventional electron energy analyzers.

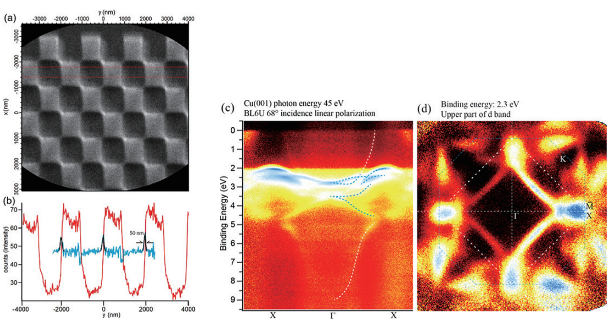

Figure 1. (a) A gold checkerboard pattern image obtained using Hg lamp. (b) Intensity profile indicating the spatial resolution of 50 nm was achieved.[1] (c) Cu valence band dispersion and iso-energy cross section.

Research Highlights

One of the highlights of the UVSOR research activities this year is the discovery of the ability of synchrotron radiation to perform coherent control.[2,3] Coherent control is a method to manipulate the populations and pathways in matters by light and is currently one of the most attractive research areas in optical physics and photochemistry. Lasers have been considered as unique light source enabling one to perform coherent control. Synchrotron radiation is usually considered as being of poor temporal coherence, therefore nobody thought that it has a hidden capability of coherent control. However, researchers have demonstrated the capability of synchrotron radiation on the coherent control using the double undulator system which is capable of producing light pulses with tailored waveform.

Figure 2 shows the schematic view of the double undulator system and the result of population control in the photoexcitation of helium atoms. The double undulator generated pairs of radiation wave packets in the extreme ultraviolet wavelength. The duration of each wave packet pair was a few femtoseconds and the time delay between them can be adjusted with attosecond precision. The individual excited states can be controlled by adjusting the interference between the electron wave packets produced in the atomic system. Moreover, the researchers succeeded also in controlling the shape and orientation of the electron cloud in a helium atom, formed as a coherent superposition state, by tuning the time delay between the circularly polarized radiation wave packets on the attosecond level.

In contrast to standard laser technology, there is no technical restriction on the extension of this method to shorter wavelengths. This new capability of synchrotron radiation not only advance the frontier of coherent control technology, but may also open up new applications in the development of functional materials and electronic devices in the future.

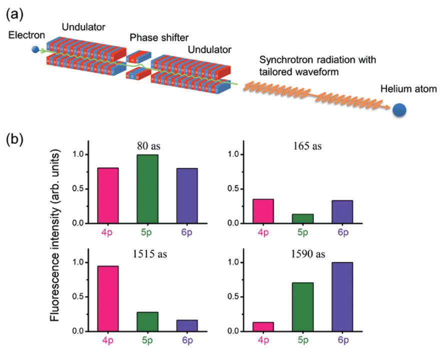

Figure 2. (a) Double undulator and produced pairs of radiation wave packets with tailored waveform. (b) Populations of 1snp states at four different time delays between the radiation wave packets.

References

1) F. Matsui *et al.*, *Jpn. J. Appl. Phys.* **59**, 067001 (2020).
2) Y. Hikosaka *et al.*, *Nat. Commun.* **10**, 4988 (2019).
3) T. Kaneyasu *et al.*, *Phys. Rev. Lett.* **123**, 233401 (2019).

Instrument Center

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SUZUKI, Toshiyasu	Team Leader
NAKAMURA, Toshikazu	Team Leader
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UEDA, Tadashi	Technical Associate
ASADA, Mizue	Technical Associate
URUICHI, Mikio	Technical Associate
OHARA, Mika	Project Manager
ISHIYAMA, Osamu	Project Manager
HASEGAWA, Hisashi	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
SHIBATA, Yuka	Secretary
ISHIKAWA, Azusa	Secretary
KATO, Kaori	Secretary
KUMITA, Machiko	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), 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). Recently, new equipment of high-performance *operando* scanning probe microscopes (Bruker Dimension XR Icon Nanoelectrical and Nanoelectrochemical, two sets) was just installed. In the fiscal year of 2019, 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 (48,827 L/year). Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute (31,751 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

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TAKADA, Noriko	Technical Associate
KIMURA, Sachiyo	Technical Associate
KIKUCHI, Takuro	Technical Associate
KIMURA, Kazunori	Technical Associate
MATSUO, Junichi	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.

Production of Detachable Models by 3D Printers

We are providing experimental tools and molecular/cellular models produced by 3D printers that use FDM (Fused Deposition Modeling), stereolithography, or binder jetting methods. The models are tools that are used by researchers to imagine molecular packing, cellular motion, *etc.* by holding them in hand. Since many researchers request to make the models detachable into multiple pieces, we have developed such models by using small magnets. 3D shape data is separated by Boolean processing so that there is no overlap between parts, and the magnets are embedded to allow each parts be reversibly detached.

A leaf primordium model in which each cell can be separated is shown in Figure 1. A Photosystem II protein model in which each subunit can be detached is shown in Figure 2.

Figure 1. Leaf Primordium model.

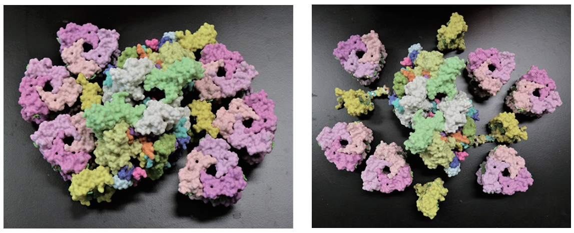


Figure 2. Photosystem II model.

NIM module Power Supply Adaptor

In experiments using a synchrotron light source or a laser, many NIM (Nuclear Instrument Modules) standard modules are used. Powers of NIM modules are supplied from BIN power supply which is expensive and heavy, even when one wishes only to put one or two NIM modules near a detector, for example.

We have developed a cheap and light-weight NIM module Power Supply Adaptor (Figure 3) which can provide power to up to two NIM modules using voltage regulator (Texas Instruments LM2941S/NOPB and LM2991S/NOPB) and AC power adaptors. It connects to NIM modules via cables and can supply maximum 1A at plus and minus 6, 12 and 24V d.c. from assigned connector pins based on the NIM standard. When it detects overcurrent, it protects own circuit and NIM modules by shutting off resettable fuses on circuit board.

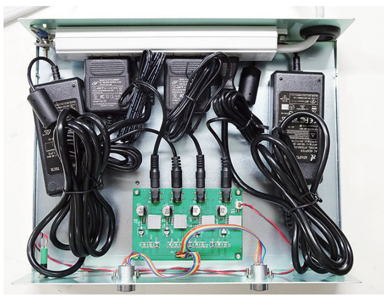


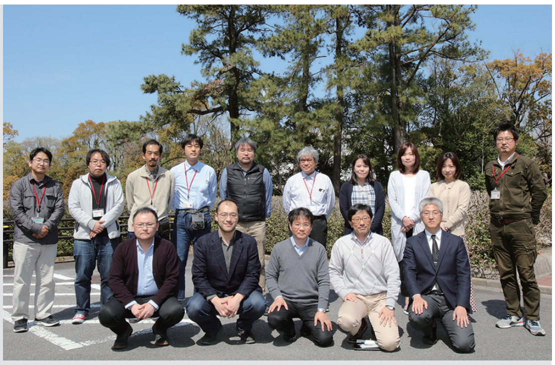
Figure 3. Inside of a NIM module Power Supply Adaptor.

Award

KONDO, Takuhiko; The Chemical Society of Japan Award for Technical Achievements for 2019.

Research Center for Computational Science (Okazaki Research Facilities)

EHARA, Masahiro	Director, Professor
SAITO, Shinji	Professor
OKUMURA, Hisashi	Associate Professor
OONO, Hitoshi	Associate Professor
ISHIDA, Tateki	Assistant Professor
UCHIYAMA, Ikuo	Assistant Professor
IWAHASHI, Kensuke	Technical Associate
MIZUTANI, Fumiyasu	Technical Associate
NAITO, Shigeki	Technical Associate
SAWA, Masataka	Technical Associate
MATSUO, Jun-ichi	Technical Associate
NAGAYA, Takakazu	Technical Associate
KAMIYA, Motoshi	Technical Associate
KINOSHITA, Takamasa	Technical Associate
UNO, Akiko	Technical Fellow
ISHIHARA, Mayumi	Secretary
KONDO, Naoko	Secretary
KONDO, Noriko	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 1,048 researchers from 268 groups in fiscal year 2019. 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.

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 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
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SAKAI, Masahiro	Technical Associate
MAKITA, Seiji	Technical Associate
MIZUTANI, Nobuo	Technical Associate
TESHIMA, Fumitsuna	Technical Associate
TSURUTA, Yumiko	Secretary
KAMO, Kyoko	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.