RESEARCH FACILITIES

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

UVSOR Synchrotron Facility

KERA, Satoshi	Director, Professor
MATSUI, Fumihiko	Professor
KATOH, Masahiro	Project Professor (Hiroshima Univ.)
TANAKA, Kiyohisa	Associate Professor
TAIRA, Yoshitaka	Associate Professor
KANEYASU, Tatsuo	Associate Professor (SAGA-LS)
ARAKI, Tohru	Senior Researcher
IWAYAMA, Hiroshi	Senior Researcher
IZUMI, Yudai	Research Lecturer
SATO, Yusuke	Assistant Professor
KATAYANAGI, Hideki	Research Associate
HAGIWARA, Kenta	IMS Fellow
MATSUDA, Hiroyuki	Post-Doctoral Fellow
SALEHI, Elham	Post-Doctoral Fellow
HAYASHI, Kenji	Engineer (Unit Leader)
NAKAMURA, Eiken	Chief Engineer
MAKITA,Seiji	Engineer
OKANO, Yasuaki	Engineer
SAKAI, Masahiro	Chief Technician
YANO, Takayuki	Chief Technician
TESHIMA, Fumitsuna	Chief Technician
KONDO, Naonori	Chief Technician
YUZAWA, Hayato	Chief Technician
OTA, Hiroshi	Technician
SHIMIZU, Kohei	Technician
MINAKUCHI, Aki	Technical Support Staff
MIZUKAWA, Tetsunori	Technical Support Staff
SUGIMOTO, Yasunobu	Technical Support Staff
YAMAZAKI, Jun-ichiro	Technical Support Staff
ISHIHARA, Mayumi	Secretary
KAMO, Kyoko	Secretary
YOKOTA, Mitsuyo	Secretary

Outline of the UVSOR Synchrotron Facility

Since the first light in 1983, the UVSOR Synchrotron Facility has been successfully operated as one of the major synchrotron light sources in Japan. After the major upgrade of accelerators in 2003, UVSOR Synchrotron was renamed to UVSOR-II Synchrotron and became one of the world's brightest low energy synchrotron light sources. In 2012, it was upgraded again and has been renamed to be UVSOR-III Synchrotron. The brightness of the electron beam was increased further. Today, six undulators are installed in total, and the storage ring, that is *ca.* 53 meters in circumference, is regularly operated in the top-up mode, irrespective of multi bunches or single bunch.

The UVSOR accelerator complex consists of a 15 MeV injector LINAC, a 0.75 GeV booster synchrotron, and a 0.75 GeV storage ring. The magnet lattice of the storage ring consists of four extended double-bend cells with distributed dispersion function. The single bunch top-up operation (176 ns, 5.6 MHz) for time-resolved measurements or low current measurements is also conducted for two weeks per year.

Six undulators and eight bending magnets provide synchrotron radiation (SR). The bending magnet, its radius of 2.2 m, produces SR with the critical energy of 425 eV. There are eight bending magnet beamlines (Table. 1). Three of the six undulators are in-vacuum soft X-ray (SX) linear-polarized undulators (BL3U, BL4U, and BL6U) and the other three are vacuum/extreme ultraviolet (VUV/XUV or EUV) circular-polarized undulators (BL1U, BL5U, and BL7U). Two beamlines, BL1U and BL6U, are so-called "in-house beamlines," which are dedicated to strategic projects conducted by internal IMS groups in tight collaboration with domestic and foreign scientists. Other twelve beamlines are so-called "public beamlines," which are open to scientists from universities, governmental research institutes, public and private enterprises, and also to overseas scientists. After each development, the in-house beamline will be opened for use as a public beamline.

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

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

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

Inter-University and International Collaboration Programs

A variety of molecular science and related subjects have been carried out at UVSOR Synchrotron Facility by IMS and external/overseas researchers. The cumulative total number of visiting researchers (person-days) per year tops > 5000, who come from > 60 different institutes. International collaborations are also pursued actively, and the number of visiting foreign researchers reaches ~70. UVSOR-III Synchrotron invites new/continuing research proposals twice a year. The proposals both for academic and public research (charge-free) and for private enterprises (charged) are acceptable. The fruits of the research activities using UVSOR-III Synchrotron are published as the UVSOR ACTIVITY REPORT annually.

Recent Developments

One of the unique UVSOR research activity is the discovery of the ability of synchrotron radiation to perform coherent control using the tandem undulator BL1U. Synchrotron radiation is usually considered as being of poor temporal coherence, therefore it is hardly thought that there is a hidden capability of coherent control. However, Katoh *et al.*, 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.[1,2]

Wave-particle duality is one of the most fundamental concepts in quantum mechanics. The concept has previously been beautifully demonstrated by the double-slit experiment, in which particles such as electrons, atoms, molecules and neutrons passing through the double-slit exhibit interference patterns in the intensity distribution on a detection screen. To produce the temporal double-slit, a tandem-undulator system is used in which each relativistic electron in the bunch emits a pair of light wave packets that has a mutual coherence between them. A pair of light wave packets sequentially interacts with a helium atom, producing a pair of photoelectron wave packets that propagate in free space and overlap each other, leading to the appearance of the interference pattern. In order to visualize the buildup of the interference pattern, the interference in the energy domain was observed (Figure 1).

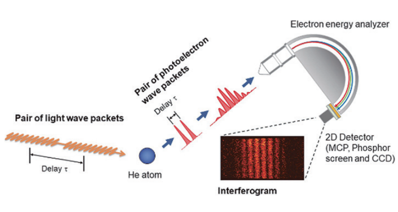

Figure 1. Time-domain double-slit experiment using a tandem-undulator system at BL1U.

Reserch Highlights

Heavy-fermion (HF) systems in rare-earth intermetallic compounds originating from the hybridization between localized *f* electrons and conduction (*c*) electrons are central topics in strongly correlated electron systems. Depending on the *c*–*f* hybridization strength at low temperatures, the ground state changes from a magnetic order to a heavy Fermi liquid. The competition between these two states makes a quantum critical point, resulting in the emergence of exotic quantum phenomena such as non-Fermi liquid and HF superconductivity. The dimensionality of the system characterizes the fundamental physical property. The combination of the HF state and low dimensionality modifies the ground state because the order parameter of these systems is much more sensitive to dimensionality. However, the monoatomic-layer Kondo-lattice showing a two-dimensional (2D) HF state has never been reported. In this study, we report the HF electronic structure of the monoatomic-layer Kondo lattice $YbCu_2$ by angle-resolved photoelectron spectroscopy (ARPES) at UVSOR-III BL5U and BL7U.[3]

Figure 2(a) shows the ARPES intensity plot around the $\bar{\Gamma}$ point at 7 K. The flat band is close to EF and highly dispersive hole bands are observed near the $\bar{\Gamma}$ point. According to the DFT calculation, the flat band and hole bands originate from the Yb^{2+} $4f_{7/2}$ and the mixing of the Yb 5*d* and Cu *sp* and *d* orbitals. The Yb^{2+} 4*f* flat band is modulated at the cross points to the conduction bands just below E_F, providing evidence of the *c*–*f* hybridization.

The temperature dependence of the quasiparticle peak just below E_F, the so-called Kondo-resonance (KR) peak, is reflected in renormalization due to the development of *c*–*f* hybridization. Figure 2(b) shows the angle-integrated (AI) photoelectron spectra as a function of temperature. The KR peak energy is shifted to the E_F with decreasing temperature, indicating the evolution of the renormalization. Figure 2(c) shows the temperature dependence of the KR peak positions. The peak position shifts with decreasing temperature and is saturated at 30 K. Such saturated temperature represents a coherence temperature (T_{coh}), at which the *c*–*f* hybridization state is fully established, resulting in a HF state.

To investigate the momentum-dependent *c*–*f* hybridization, we took the temperature-dependent peak position of the KR peak at three wavenumbers (k_x = 0.5, 0.0, −0.1 Å^{-1}) (not shown). The change of the peak position at k_x = 0.5 Å^{-1} almost follows the AI one. In contrast to the saturated feature in the AI spectrum at T = 30 K, the KR peak positions at k_x = 0.0 and −0.1 Å^{-1} are shifted to the higher-binding energy side below T_{coh}, suggesting the hybridization gap enlargement.

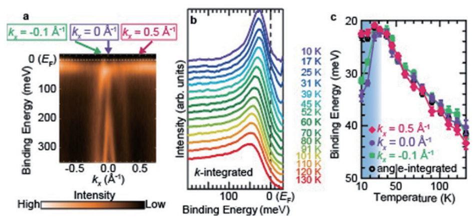

Figure 2. (a) The ARPES intensity plot around $\bar{\Gamma}$ point taken with horizontally polarized 37 eV photons at 7 K. (b) Angle-integrated photoelectron spectra as a function of temperature taken with horizontally polarized 35 eV photons. (c) Momentum dependence of the energy position of the quasiparticle peak plotted on a linear temperature scale.

References

1) Y. Hikosaka *et al.*, *Nat. Commun.* **10**, 4988 (2019); **12**, 3782 (2021).
2) T. Kaneyasu *et al.*, *Sci. Rep.* **12**, 9682 (2022).
3) T. Nakamura *et al.*, *Nat. Commun.* **14**, 7850 (2023).

Instrument Center

YOKOYAMA, Toshihiko	Director, Professor
SUZUKI, Toshiyasu	Team Leader
NAKAMURA, Toshikazu	Team Leader
MINATO, Taketoshi	Senior Researcher
SHIGEMASA, Eiji	Unit Leader
TAKAYAMA, Takashi	Chief Engineer
FUJIWARA, Motoyasu	Chief Technician
UEDA, Tadashi	Chief Technician
ASADA, Mizue	Chief Technician
OKANO, Yoshinori	Technician
URUICHI, Mikio	Technician
MIYAJIMA, Mizuki	Technician
NAGAO, Haruyo	Technician
HIRANO, Kaho	Technician
MINAMINO, Yu	Technician
ISHIYAMA, Osamu	Project Manager
NAKAMOTO, Keiichi	Project Manager
OTA, Yasuhito	Project Manager
KAKU, Mie	Project Manager
OHARA, Mika	Research Fellow
IKI, Shinako	Technical Associate
ISHIDA, Himawari	Technical Associate
FUJIKAWA, Kiyoe	Technical Support Staff
KUBOTA, Akiko	Technical Support Staff
IMAI, Yumiko	Technical Support Staff
UCHIDA, Mariko	Technical Support Staff
IWASE, Mahiro	Technical Support Staff
FUNAKI, Yumiko	Secretary
HYODO, Yumiko	Secretary
KURITA, Yoshiko	Secretary
TOYAMA, Yu	Secretary

Instrument Center was organized in April of 2007 by integrating the general-purpose and state-of-the-art facilities of Research Center for Molecular Scale Nanoscience and Laser Research Center for Molecular Science. The mission of Instrument Center is to support 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, JNM-ECZL 600, and JNM-ECS400 for solutions), matrix assisted laser desorption/ionization time-of-flight (MALDI TOF) mass spectrometer (microflex LRF, Bruker Daltonics), ESI-TOF mass spectrometer (Bruker Daltonics, maXis), powder X-ray diffractometer (Rigaku RINT-Ultima III), molecular structure analysis using crystalline sponge method (Rigaku SuperNova), circular dichroism (CD) spectrometer (JASCO J-1500), differential scanning calorimeter (MicroCal VP-DSC), isothermal titration calorimeter (MicroCal PEAQ-iTC & iTC200), field emission transmission electron microscope (JEOL JEM-2100F), elemental analyzer (J-Science Lab Micro Corder JM10), ICP atomic emission spectroscopy (Agilent 5110 ICP-OES), fluorescence spectrometer (JASCO FP-8650DS), fluorescence lifetime spectrometer (Quantaurus-Tau C16361-01), electron probe microanalyzer (EPMA, JEOL JXA-8230/SS-94000SXES), and automatic organic molecular synthesis (Cole-Parmer reaction station Integrity 10).

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

In the fiscal year of 2023, Instrument Center accepted 141 applications from outside and the total user time amounted 2,072 days for outside and 925 days for in-house. Instrument

Center also maintains helium liquefiers in the both campus and provides liquid helium to users (52,706 L/year). Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute (45,153 L/year).

Instrument Center also organizes the Inter-University Network for Common Utilization of Research Equipments 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.

Award

NAGAO, Haruyo; ARIM Japan The Best Technical Support Contribution Award (2024).

Equipment Development Center

YAMAMOTO, Hiroshi	Director
KONDO, Takuhiko	Chief Engineer (Unit Leader)
TOYODA, Tomonori	Chief Engineer
MATSUO, Junichi	Chief Technician
TAKADA, Noriko	Chief Technician
KIMURA, Sachiyo	Technician
KIKUCHI, Takuro	Technician
KIMURA, Kazunori	Technician
MIYAZAKI, Yoshino	Technician
ISOGAI, Toshifumi	Technician
SAWADA, Toshihiro	Technical Support Staff
ISHIKAWA, Akiko	Technical Support Staff
SUGANUMA, Kouji	Technical Support Staff
INAGAKI, Itsuko	Secretary

Research and development of novel instruments demanded in the forefront of molecular science, including their design and fabrication, are the missions of this center. Technical staffs in the three work sections, mechatronics, electronics and lithography are engaged in developing state-of-the-art experimental instruments in collaboration with scientists. We expanded our service to other universities and research institutes since 2005, to contribute to the molecular science community and to improve the technology level of the center staffs. A few selected examples of our recent developments are described below.

Introduction of New Lithography Equipment

Several types of lithography equipment have been installed in our clean room over the past few years.

One is a Reactive Ion Etching (RIE) machine, the "RIE-10NR" from Samco Inc. This machine can etch silicon (Si) and silicon dioxide (SiO_2) using carbon tetrafluoride gas as a process gas, and it can also etch organic materials using O_2 gas (Figure 1 left). Before this equipment was installed, we performed wet etching using corrosive solutions. With the installation of the RIE equipment, dry etching is now possible, allowing us to fabricate finer patterns that were previously unachievable with wet etching.

Another piece of equipment is the Evaporation Equipment, which was donated to us by a research group at the Institute for Molecular Science. It is a customized version of ULVAC's Compact Evaporation Equipment DEPOX Series "VTS-350M/ERH." Since the equipment was not ready for immediate use after relocation, members of the Equipment Development Center collaborated to set it up. We have successfully confirmed that gold can be deposited using this system (Figure 1 right).

We plan to use the aforementioned equipment extensively for microfabrication *via* lithography.

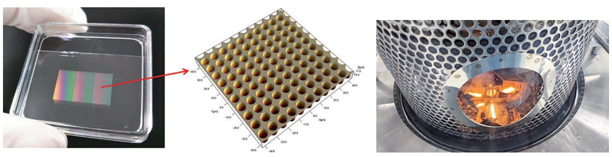

Figure 1. Examples of fabrication using O_2 gas as a process gas (left) and gold evaporation (right).

Electronics Instruments for Low-Temperature Scanning Near-Field Optical Microscopy

By utilizing near-field techniques, scientists can perform optical imaging and spectroscopy below the diffraction limit. To achieve near-field optical measurements at ultra-low temperatures and ultra-high vacuum conditions, we have developed three electronic instruments: (1) an interferometer that precisely detects and amplifies interference light generated in optical fibers; (2) an instrument that provides feedback signals based on fluctuations in the distance between the optical fiber and cantilever; (3) a driver that moves the piezo stage to fine-tune these fluctuations. Since we detect, amplify, and control weak signals, all instruments are constructed entirely with analog circuits.

The interferometer detects interference light from the optical fiber using a four-quadrant photodiode and amplifies it 250,000 times using a detection circuit built with ADA4627-1ARZ (Analog Devices). The feedback instrument smooths and holds fluctuations of less than 10 Hz, which are mixed in the interference light, using an integrating circuit with ADA4084-1ARZ (Analog Devices). The driver, constructed primarily with a high-voltage amplifier PA441DF (Apex), drives the piezo stage to fine-tune the fluctuation correction (Figure 2).

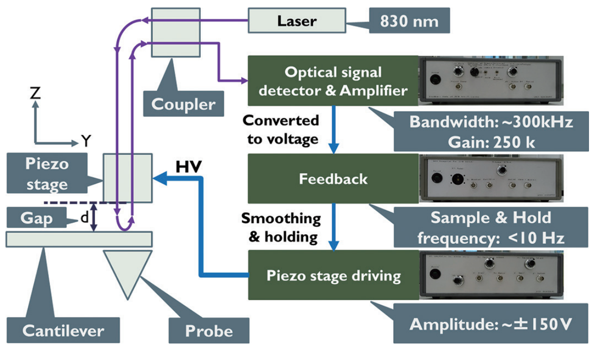

Figure 2. Schematic of electronics instruments for NCAFM (Non-Contacting Atomic Force Microscope) based on optical fiber detection.

Research Center for Computational Science (Okazaki Research Facilities)

EHARA, Masahiro	Director, Professor
SAITO, Shinji	Professor
OKUMURA, Hisashi	Associate Professor
OKAZAKI, Kei-ichi	Associate Professor
OONO, Hitoshi	Associate Professor
UCHIYAMA, Ikuo	Associate Professor
OHNUKI, Jun	Assistant Professor
SHIRAOGAWA, Takafumi	Assistant Professor
ISHIDA, Tateki	Research Associate
IWAHASHI, Kensuke	Chief Engineer (Unit Leader)
MIZUTANI, Fumiyasu	Engineer
NAITO, Shigeki	Chief Technician
KAMIYA, Motoshi	Chief Technician
SAWA, Masataka	Technician
NAGAYA, Takakazu	Technician
KINOSHITA, Takamasa	Technician
SUZUKI, Kazuma	Technician
KANESHIRO, Ikuma	Technician
YAZAKI, Toshiko	Technical Associate
UNO, Akiko	Technical Support Staff
KONDO, Noriko	Secretary
URANO, Hiroko	Secretary

Research Center for Computational Science provides state-of-the-art computational resources to academic researchers in molecular science and related fields, *e.g.* solid state physics, biophysics, basic biology, and physiology. Our systems consist of HPE Apollo 2000 and Apollo 6500 (since Feb. 2023). The combined system, named "Molecular Simulator," is ranked 196th position in the TOP500 supercomputer list in June 2023. These massive computer resources have been used for various kinds of large-scale calculations, for example accurate electronic structure calculations of molecular systems and conformation searches using non-Boltzmann ensemble methods. We also provide about 30 application programs to the users: Gaussian, GAMESS, Molpro, AMBER, Gromacs, and so on. In particular, we have implemented some original programs developed by researchers in Japan to provide them to the users. The supercomputer systems had been used by 1,315 researchers from 302 groups in the fiscal year 2023. 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 2023, the numbers of registered attendants of these schools were 329 and 380, 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 2023, we organized the workshop under the title, "Frontiers of Biomolecular Science based on Simulations, Informatics, and AI."

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

We also offer Quantum Chemistry Literature Database (QCLDB; http://qcldb2.ims.ac.jp/), Force Constant Database (FCDB; http://fcdb.ims.ac.jp/), and Segmented Gaussian Basis Set (SGBS; http://sapporo.center.ims.ac.jp/sapporo/) services. The latest release, QCLDB II Release 2016, containing 139,657 data of quantum chemical studies is available for the registered users. FCDB provides force constants of molecules collected from literature. SGBS service provides basis sets for atoms which efficiently incorporate valence and core electron correlations (also known as Sapporo basis sets) in various quantum chemistry package formats. Further details about the hardware, software, and the other services are available on our website (English: https://ccportal.ims.ac.jp/en/, Japanese: https://ccportal.ims.ac.jp/).

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

Figure 1. HPE Apollo 2000 and Apollo 6500.