RESEARCH FACILITIES

The Institute includes five research facilities. This section describes their latest equipment and activities. For further information please refer to older IMS Annual Review issues (1978–2007).
Outline of UVSOR

The UVSOR accelerator complex consists of a 15 MeV injector linac, a 600 MeV booster synchrotron, and a 750 MeV storage ring. The magnet lattice of the storage ring is the so-called double-bend achromat. The double RF system is routinely operated for the user beam time, and the lifetime of the electron beam has been improved to around 6 hours at 200 mA. The storage ring is normally operated under multi-bunch mode with partial filling. The single bunch operation is also conducted about two weeks per year, which provides pulsed synchrotron radiation (SR) for time-resolved experiments. Initial beam currents stored under multi-bunch and single-bunch modes are 350 mA and 70 mA, respectively.

Eight bending magnets and three insertion devices are available for utilizing SR. The bending magnet with its radius of 2.2 m provides SR, whose critical energy is 425 eV. After completing the upgrade project, there are 14 beamlines available in total (13 operational, and 1 under construction) at UVSOR, which can be classified into two categories. 9 of them are the so-called “Open beamlines,” which are open to scientists of universities and research institutes belonging to the government, public organizations, private enterprises and those of foreign countries. The rest of the 5 beamlines are the so-called “In-house beamlines,” which are dedicated to the use of the research groups within IMS. We have 1 soft X-rays (SX) station equipped with a double-crystal monochromator, 8 EUV and SX stations (one of them is under construction) with a grazing incidence monochromator, 3 VUV stations with a normal incidence monochromator, 1 (far) infrared station equipped with FT interferometers, 1 station with a multi-layer monochromator.

Collaborations at UVSOR

Variety of investigations related to molecular/material science is carried out at UVSOR by IMS researchers. In addition, many researchers outside IMS visit UVSOR to conduct their own research work. The number of visiting researchers per year tops about 800, whose affiliations extend to 60 different institutes. International collaboration is also pursued actively and the number of visiting foreign researchers reaches over 80, across 10 countries. UVSOR invites new/continuing proposals for research conducted at the open beamlines twice a year. The proposals from academic and public research organizations (charge-free) and from enterprises (charged) are acceptable. The fruit of the research activities using SR at UVSOR is published as a UVSOR ACTIVITY REPORT annually. The refereed publications per year count more than 60 since 1996. In recent five years, the number of beamlines has been reduced from 22 to 14. The upgrade project of the UVSOR storage ring, in which the creation of four new straight sections and the achievement of much smaller emittance (27 nm-rad) were planned in 2002–2003, has been accomplished on schedule. The upgraded storage ring is named UVSOR-II. The numbers of users and related publications have shown an upward tendency, since 2004.
Highlights of Users’ Researches 2007

1) Infrared Reflection-Absorption Spectroscopy of Alq3 Thin Film on Silver Surface Using Synchrotron Radiation

Y. Sakurai, S. Kimura, K. Seki (UVSOR, Nagoya Univ.)

Recently, organic semiconductors are attracting attention because of possible applications to electronic devices such as organic light emitting diodes (OLEDs). In OLEDs, tris(8-hydroxyquinoline) aluminum (Alq3) is most widely used as the electron transport/light emitting material. Alq3 has two possible geometrical isomers of meridional (C1 symmetry) and facial (C3 symmetry) forms. It is important to find whether facial isomer exists at the interface between the metal and the Alq3 film or not.

Vibrational spectroscopy such as infrared (IR) spectroscopy is a suitable technique for distinguishing these isomers. We examined whether the facial isomer exists at the interface between the Ag and the Alq3 film or not by infrared reflection-absorption spectroscopy (IRAS) using a synchrotron radiation (SR) light source. Use of highly brilliant infrared synchrotron radiation (IRSR) source enables us to obtain IRAS spectra in the low wavenumber region, which cannot be covered by conventional IRAS system using globar light source because of its low brilliance.

Figure 2 indicates the thickness dependence of the IRAS spectra of an Alq3 film deposited on an Ag surface. The observed IRAS spectra suggest that the Alq3 film predominantly consists of meridional isomer including the first monolayer adsorbed on the Ag surface. In the spectrum of monolayer Alq3, Al–N stretching mode slightly shifts to the lower wavenumber side than that of multilayer Alq3, possibly due to the charge transfer between the Alq3 and Ag surface.

Figure 2. The thickness dependence of the IRAS spectra of an Alq3 film on Ag surface.

2) Electronic Structure at Highly Ordered Organic/Metal Interfaces

H. Yamane, K. Kanai, K. Seki (Nagoya Univ.)

The electronic structure at the interface formed between an organic semiconductor film and a metal electrode plays a crucial role in the performance of electronic devices using organic semiconductors such as electroluminescent displays, field-effect transistors, and photovoltaic cells.

We have studied the electronic structure of well-ordered thin films of pentacene (Pn) molecules prepared on Cu(110) in the monolayer regime, by using angle-resolved UV photoemission spectroscopy. The Pn molecules on Cu(110) in the monolayer regime form a highly ordered film structure with planar adsorption geometry, where the molecular long axis is parallel to the [110] substrate direction.

Figure 3(a) and (b) shows the observed energy versus momentum [E(k)] relation for the flat-lying Pn monolayer film on Cu(110) along (a) φ = 0° (the [110] substrate direction) and (b) φ = 28°. The selected raw ARUPS spectra of the valence levels and the secondary-electron cutoff are shown in Figure 3(c) and (d), respectively.

We found that the change in the work function upon the adsorption of the flat-lying Pn monolayer film is Δω = –0.9 eV [Figure 3(d)] due to the formation of the interfacial dipole layer. We clearly observed the electronic structure characteristic of the interface with the following findings: (i) formation of the interface states with possible modification of the orbital symmetry and the energy position, and (ii) two-dimensional inter-molecular band dispersion of these interface states with the effective mass of the hole for the upper branch being 0.24 m0 at 300 K.

Figure 3. (a,b) E(kφ) relation for the highly ordered flat-lying Pn monolayer film on Cu(110) at φ = (a) 0° and (b) 28°. Open and filled circles indicate the position of the Pn-derived peaks measured at hν = 20 and 30 eV, respectively. (c,d) Selected ARUPS spectra of the Pn monolayer film and the bare substrate for the regions of (c) valence levels and (d) secondary-electron cutoff.

* Present Address; JASRI
Research Center for Molecular Scale Nanoscience

Research Center for Molecular Scale Nanoscience was established in 2002 with the mission of undertaking comprehensive studies of “Molecular Scale Nanoscience.” The Center consists of one division staffed by full-time researchers (Division of Molecular Nanoscience), two divisions staffed by adjunctive researchers (Divisions of Instrumental Nanoscience and Structural Nanoscience), one division staffed by visiting researchers (Division of Advanced Molecular Science). Their mandates are

1) Fabrication of new nanostructures based on molecules
2) Systematic studies of unique chemical reactions
3) Systematic studies of physical properties of these nanostructures.

The Center administers offers public usage of the advanced ultrahigh magnetic field NMR (Nuclear Magnetic Resonance, 920 MHz) spectrometer not only for solution specimens but for solid samples. Since 2004 a number of collaborating researches with the 920 MHz NMR measurements have been examined. Figure shows the apparatus, together with a typical example of the NMR spectra, where one can easily find much better resolving power than that of a standard 500 MHz NMR spectrometer. (1) dynamic structures of biological macromolecules, (2) structure of bioactive natural products, (3) characterization of metal ion complexes and so forth. We will continuously call for the collaborating research applications using the 920MHz NMR spectrometer with a view to use the NMR of a wide scientific tolerance (e.g., structural biology, organic chemistry, catalyst chemistry, etc.).

Since 2005, Nanoforum has been organized, which supports small international/domestic meetings and seminars related to nanoscience. The Center also conducts the Nanotechnology Network Project of the Ministry of Education, Culture, Sports, Science and Technology (MEXT) as a core organization, and provides various kinds of nanotechnology public support programs to Japanese and foreign researchers. This project will be described in the other section in this book.

Figure 1. 920 MHz NMR spectrometer and an example measured using 920 and 500 MHz spectrometers. Much higher resolution in 920 MHz can be clearly seen.

* from Nagoya City University
† from JEOL Datum
Laser Research Center for Molecular Science

The center aims to develop new experimental apparatus and methods to open groundbreaking research fields in molecular science, in collaboration with the Department of Photo-Molecular Science. Those new apparatus and methods will be served as key resources in advanced collaborations with the researchers from the community of molecular science. The main targets are (1) advanced photon sources covering wide energy ranges from terahertz to soft X-day regions; (2) novel quantum-control schemes based on intense and ultrafast lasers; and (3) high-resolution optical imaging and nanometric microscopy. The center also serves as the core of the joint research project “Extreme Photonics” between IMS and RIKEN.

Figure 1. Microchip laser developed at the center.

Figure 2. Theoretical simulation of quantum interferometric images generated in a single molecule with a pair of two laser pulses whose timing is controlled on the attosecond ($10^{-18}$ sec) timescale.
**Instrument Center**

Instrument Center was organized in April of 2007 by integrating the general-purpose 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 are conducting their researches using general-purpose instruments such as ESR, x-ray diffractometer, fluorescence spectrometer, etc. The staffs of Instrument Center maintain the best condition of the machines, and provide consultation for how to use them. The main instruments are NMR (JEOL JNM-LA500, JEO JNM-LA400), mass spectrometer (Voyager DE-STR), powder x-ray diffractometer (Rigaku RINT-Ultima III), and circular dichroic spectrometer (JASCO JW-720W1) in Yamate campus and ESR (Bruker E680, E500, EMX Plus), SQUID magnetometer (Quantum Design MPMS-7, MPMS-XL7minTK), powder (MAC Science MXP3) and single-crystal (Rigaku Mercury CCD, RAXIS IV, 4176F07) diffractometer, dilution refrigerator (Oxford 400µ) with superconducting magnet (12 T), thermoanalysis system (TA TGA2950, DSC2920, SDT2960), fluorescence spectrophotometer (SPEX FluorogII), UV-VIS-NIR (Hitachi U-3500) spectrophotometer, excimer+dye laser (LPX105i), Nd-YAG+OPO laser (GCR-250), and excimer laser (Complex 110F) in Myodaiji campus. Instrument Center provides liquid nitrogen and liquid helium using helium liquefiers. The staffs of Instrument Center provide consultation for how to treat liquid helium, and provide various parts necessary for low-temperature experiments. Instrument Center supports also the network sharing system of the chemistry-oriented instruments, which started in the April of 2007. In the fiscal year of 2007 (April 2007 to March 2008), Instrument Center accepted 27 applications from 27 institutions outside of IMS. The users mainly used SQUID (15), ESR (18), x-ray diffractometer (21), mass spectrometer (2), NMR (3), and Excimer-dye laser (2), where the numbers in parenthesis shows the number of use by external users.

**Figure 1.** High-Frequency/High-Field ESR Spectrometer (Bruker E680).

**Figure 2.** Matrix-Assisted Laser Desorption Ionization—Time of Flight Mass Spectrometer (Applied Biosystems Voyager DE-STR).

**Figure 3.** Excimer+dye laser (Lambda physics LPX 105i + LPD3002).
Design and fabrication including the research and developments of the new instruments necessary for the molecular science are the mission of this center, which consists of the mechanical, electronics and glass work sections. We expanded our service to the outside researchers of universities and research institutes since 2005. The main aims of this new attempt are to contribute to the molecular science community and to improve the technology level of the center staffs.

The technical staff of the Equipment Development Center is engaged in planning, researching, designing and constructing high technology experimental instruments in collaboration with the scientific staff. And these experimental instruments are manufactured by incorporating with new technologies and new mechanical ideas. A part of our activity in the current fiscal year is described below.

Development of a Cell for a Gas-Phase Nuclear Magnetic Resonance Spectrometer

This project was proposed by Prof. Fuke (Department of Chemistry, Kobe University), who is developing a gas-phase NMR spectrometer. The apparatus was selected in System Development Program for Advanced Measurement and Analysis of JST (Development of Systems and Technology for Advanced Measurement and Analysis) in 2007, and it was adopted as the institution use of the latter period in 2007.

NMR spectroscopy is widely used for liquid and solid samples. The aim of the development is to extend the NMR application to the gaseous ions. The system consists of a FT ICR (ion cyclotron resonance) mass analyzer and a NMR spectrometer, and provides us NMR data of mass-selected ions. It is expected to be available with the gas phase molecular ions ($m/e < 2000, < 10^5 /cm^3$).

In this project, the NMR cell, which is mounted in 12T magnet, was designed and constructed. Since the magnetic bore ( $\phi 155 \text{ mm} \times 2000 \text{ mm}$) is long and spatially limited, there are several difficult points for designing the cell. Figure 1 shows the schematic design of NMR cell. In order to trap slow-velocity ions in the NMR cell, the electrical noise aroused from RF magnetic fields must be efficiently suppressed. To overcome this problem, the electric wires were introduced through inside of the pipes which support the cell mechanically. A technical development was also required to mount a Cu mesh (95% transparency) on the NMR-cell electrodes. In addition to these, there are several technical problems, which we are now overcoming.

In this program, Mr. Horigome, who is the staff of UVSOR Facility, also cooperated to accomplish this joint development project. Because he has enough experience of making vacuum machinery.

We had several meetings with the researchers of Kobe University and discussed on the design of the cell. The NMR cell is going to be constructed in the latter period in 2008.

Fabrication of a Precision CNC Milling Machine

In recent years, micro fluidic channel is rapidly becoming important tools in wide science technology fields such as analytical chemistry and medical biology. The pattern of micro channels is usually fabricated by the photolithography. However, the photolithographic method requires complex chemical and mechanical processes and expensive photomasks. It is difficult to make a deep channel, and waste fluid processing an intractable problem. Due to these disadvantages of photo-
lithographic method, importance of micromachining by cutting is becoming important. In relation to this, machine tool companies are selling various micro machinery tools. Moreover, needs for micromachining is also increasing in IMS. Based on these requirements, we started the developments of micromachining technology several years ago. However, since it is difficult to make precise microstructures by using old type machine due to large cutting errors, we decided to fabricate a precise CNC milling machine. As shown in Figure 2, this machine consists of a spindle, the xyz submicron stage and a substance microscope. We fixed the spindle to an auto collimator base which is used for coarse control. As shown in Figure 3, we made a mask for synchrotron radiation etching by using this machine. This mask has 25 through holes in a plate with 30 µm thickness. We thought it was difficult to make this by using our old type machine, and the importance of the new type of precise machinery has been demonstrated.

Figure 2. Newly developed Precision CNC milling machine.

Figure 3. Mask for synchrotron radiation etching.
Research Center for Computational Science

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EHARA, Masahiro  
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ISHIDA, Tateki  
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NAITO, Shigeki  
SAWA, Masataka  
IWASHI, Kento  
MATSUO, Jun-ichi  
NAGAYA, Takahiro  
TOYA, Akiko  
ISHIHARA, Mayumi  

Director, Professor  
Professor  
Professor  
Assistant Professor  
Assistant Professor  
Assistant Professor  
Technical Associate  
Technical Associate  
Technical Associate  
Technical Associate  
Technical Associate  
Technical Associate  
Secretary  
Secretary

Research Center for Computational Science, Okazaki Research Facilities, National Institutes of Natural Sciences, provides state-of-the-art computational resources and software to academic researchers in molecular science and related fields. The Center currently has over 600 users in 145 project groups from a wide range of molecular science, i.e. quantum chemistry, molecular simulation, chemical reaction dynamics and solid state physics. In order to meet a wide variety of users’ demands, the computer systems consist of Fujitsu PRIMEQUEST, SGI Altix4700, and Hitachi SR-16000. These systems are linked to Internet through Science Information Network (SINET3).

The Center provides a number of state-of-the-art application programs, including Gaussian 03, GAMESS, Molpro, AMBER, NAMD, etc.; which are installed to the computer systems and kept updated for immediate use of the users. The Center also maintains and offers the Quantum Chemistry Literature Database (QCLDB, http://qclpdb2.ims.ac.jp/), which has been developed by the Quantum Chemistry Database Group in collaboration with staff members of the Center. The latest release, QCLDB II Release 2007, contains 97,718 data of quantum chemical studies. Detailed information on the hardware and software at the Center is available on the web site (http://ccinfo.ims.ac.jp/).

In addition to offering computer resources to molecular scientists, another vital aspect of the Center is to perform leading computational researches with massive computations. In 2003, the Center joined the National Research Grid Initiative (NAREGI) project, a three-year national project by National Institute of Informatics (NII) and IMS. This joint project aimed at developing grid computing system (NII) and thereby realizing extremely large-scale computational studies in the frontier of nanoscience (IMS). For these purposes, two supercomputer systems, Hitachi SR11000 and HA8000, were introduced to the Center in 2004, with combined performance exceeding 10 TFlops. In 2006, the NAREGI project was reformed to join a new national project Development and Application of Advanced High-Performance Supercomputer Project by RIKEN, where IMS plays an important role in the application of the PFlops-scale supercomputer to nanoscience. Further information on next-generation supercomputer project and computer systems at the Center is found on the web site (http://ims.ac.jp/nanogrid/).

Figure 1. Super-High-Performance Molecular Simulator.
Okazaki Institute for Integrative Bioscience

The main purpose of Okazaki Institute for Integrative Bioscience (OIIB) is to conduct interdisciplinary, molecular research on various biological phenomena such as signal transduction, differentiation and environmental response. OIIB, founded in April 2000, introduces cutting edge methodology from the physical and chemical disciplines to foster new trends in bioscience research. OIIB is a center shared by and benefited from all three institutes in Okazaki, thus encouraging innovative researches adequately in advance of academic and social demands. The research groups of three full professors and one associate professor who have the position in IMS join OIIB. The research activities of these groups are as follows.

Aono group is studying the bioinorganic chemistry of hemeproteins that show a novel function. They solved the structure and function relationships of the CO sensor protein CooA and O₂ sensor protein HemAT. They also reported the structure and function relationships of aldoxime dehydratase, which is a novel heme-containing dehydrase enzyme. Kato group is studying structure, dynamics, and interactions of biological macromolecules primarily using ultra-high field nuclear magnetic resonance (NMR) spectroscopy. In particular, they conducted studies aimed at elucidating the dynamic structures of glycoconjugates and proteins for integrative understanding of the mechanisms underlying their biological functions. Kuwajima group is studying mechanisms of in vitro protein folding and mechanisms of molecular chaperone function. Their goals are to elucidate the physical principles by which a protein organizes its specific native structure from the amino acid sequence. In this year, they studied the equilibrium and kinetics of canine milk lysozyme folding/unfolding by peptide and aromatic circular dichroism and tryptophan fluorescence spectroscopy. Fujii group is studying molecular mechanisms of metalloenzymes, which are a class of biologically important macromolecules having various functions such as oxygen transport, electron transfer, oxygenation, and signal transduction, with synthetic model complexes for the active site of the metalloenzymes. In this year, they studied molecular mechanisms of metalloenzymes relating to monoxygenation reactions and denitification processes.

OIIB is conducting the cooperation research program, “Frontiers of Membrane Protein Research,” with Institute for Protein Research, Osaka University from 2005. In this program, the following projects have being carried out to elucidate the role of membrane proteins in life: (i) the development of expression systems, purification methods, and chemical synthesis of membrane proteins, (ii) the development of new methods for analyzing the structure and function of membrane proteins. As a part of this cooperation program, International Symposium on Membrane Protein Research—Perspective in Structural Biology of Membrane Proteins and Biological Macromolecules was held in Osaka on March 22, 2008.
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 comprised 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.