RESEARCH FACILITIES

The Institute includes five research facilities. This section describes their latest equipment and activities. For further information please refer to previous IMS Annual Review issues (1978–2010).

UVSOR Facility

KATOH, Masahiro	Director, Professor
SHIGEMASA, Eiji	Associate Professor
KIMURA, Shin-ichi	Associate Professor
ADACHI, Masahiro	Assistant Professor
ZEN, Heishun	Assistant Professor
IWAYAMA, Hiroshi	Assistant Professor
MATSUNAMI, Masaharu	Assistant Professor
OHIGASHI, Takuji	Assistant Professor
HORIGOME, Toshio	Technical Associate
NAKAMURA, Eiken	Technical Associate
YAMAZAKI, Jun-ichiro	Technical Associate
HASUMOTO, Masami	Technical Associate
SAKAI, Masahiro	Technical Associate
HAYASHI, Kenji	Technical Associate
KONDO, Naonori	Technical Associate
TOKUSHI, Tetsunari	Technical Fellow
HAGIWARA, Hisayo	Secretary

Outline of UVSOR

After the major upgrade in 2003, UVSOR was renamed to UVSOR-II and became one of the world brightest low energy synchrotron light source. The UVSOR accelerator complex consists of a 15 MeV injector linac, a 750 MeV booster synchrotron, and a 750 MeV storage ring. The magnet lattice of the storage ring consists of four extended double-bend cells with distributed dispersion function. Since July, 2010, the storage ring has been operated for users fully in so-called top-up mode, in which the electron beam intensity is kept almost constant at 300 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.

Eight bending magnets and four undulators are available for utilizing SR. The bending magnet with its radius of 2.2 m provides SR with the critical energy is 425 eV. There are 12 beam-lines operational at UVSOR, which can be classified into two categories. 8 of them are the so-called "Open beam-lines," which are open to scientists of universities and research institutes belonging to the government, public organizations, private enterprises and those of foreign countries. The other 4 beam-lines 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, 7 EUV and SX stations with a grazing incidence monochromator, 3 VUV stations with a normal incidence monochromator, 1 (far) infrared station equipped with FT interferometers.

Figure 1. Overview of the UVSOR storage ring room.

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.

Recent Developments of the Facility 2010

We have started operating the machine in the top-up injection mode for 100% of the users' beam time since the fiscal year 2010, both in the multi- and single-bunch operations. The beam current is kept approximately constant at 300 mA for the multi-bunch mode. As a result, the average beam current increased by about 40%, comparing with that of the previous year, as shown in Figure 2.

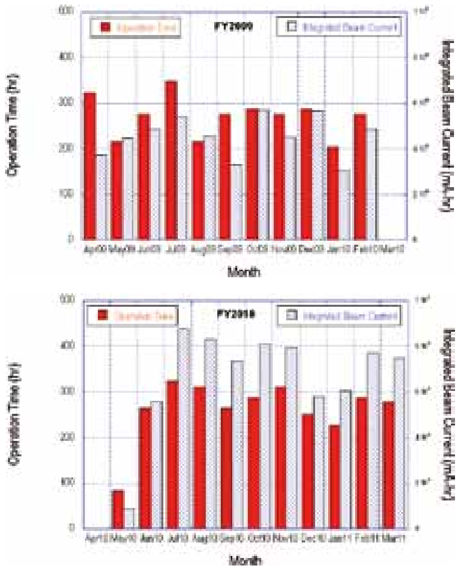


Figure 2. Monthly Statistics of UVSOR Operation. The red bars are for the operation time (hr) and the blue-hatched bars are for the integrated beam current (mA-hr). The increase of the integrated beam current is significant while the operation time did not increase so much, comparing with FY2009 (upper) and FY2010 (lower).

In spring 2010, we have installed a new undulator, which will be used for light source developments under the support of Quantum Beam Technology Program by MEXT. New dedicated beam lines to extract coherent synchrotron radiation in THz and VUV range are under construction. To realize this, two operational beam lines were moved to other sections, and one of them has been completely renewed.

A new upgrade program is in progress, in which all eight bending magnets will be replaced to reduce the emittance more. One new undulator will be installed at the last straight section reserved for an insertion device. A novel EUV micro-spectroscopy beam line will be constructed. This upgrade will be completed in summer 2012. Then, we will call our machine UVSOR-III.

Reserch Highlight 2010

Nodeless Superconducting Gap in $A_xFe_2Se_2$ (A = K, Cs) Revealed by Angle-Resolved Photoemission Spectroscopy

Recently, a new series of iron-based superconductors, $A_xFe_2Se_2$ (A = K, Cs), has been discovered with relatively high transition temperature of ~30 K.[1] Angle-resolve photoemission spectroscopy experiment on $A_xFe_2Se_2$ (A = K, Cs) was conducted at BL7U.[2]

Figure 3 (a) reveals the photo emission intensity map along out-of-plane momentum (k_z) in the ΓZAM plane. The cross-sections of the κ and δ Fermi surfaces clearly show weak dispersion along the k_z direction, indicative of a rather two-dimensional electronic structure. The spectral weight of κ increases from Γ to Z, and a small electron pocket could be clearly observed for the κ band around Z [Fig. 3 (b)]. This gives an electron pocket around Z with its residual spectral weight extending towards Γ. However, we emphasize that the size of the κ pocket is much smaller than that of the δ pocket, which is rather k_z-independent. The experimental Fermi surface topology clearly shows that there is no hole Fermi surface near the zone center, and $A_{0.8}Fe_2Se_2$ is indeed the most heavily electron-doped iron-based superconductor by far.

Our data show that the rather robust superconductivity in such a highly electron-doped iron-based superconductor could mainly rely on the electron Fermi surfaces near M. Thus, the sign change in the $s_\pm$ pairing symmetry driven by the inter-band scattering as suggested in many weak coupling theories becomes conceptually irrelevant in describing the superconducting state here. A more conventional s-wave pairing is probably a better description.

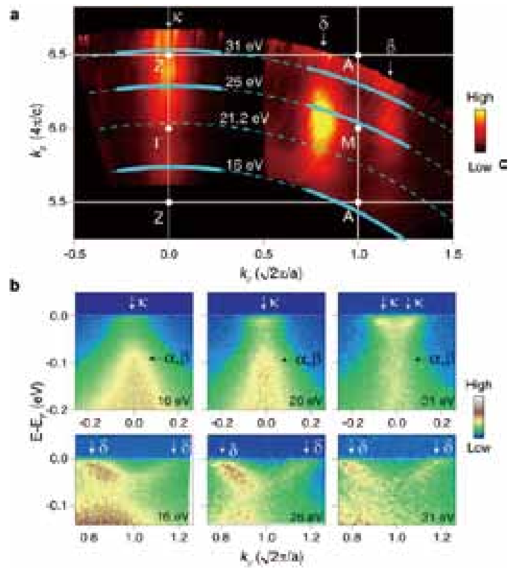


Figure 3. The Fermi surface and band structure as a function of k_z for $K_{0.8}Fe_2Se_2$.

References

1) J. Guo *et al.*, *Phys. Rev. B* **82**, 180520 (2010).

2) Y. Zhang *et al.*, *Nat. Mater.* **10**, 273 (2011).

Research Center for Molecular Scale Nanoscience

YOKOYAMA, Toshihiko	Director, Professor
HIRAMOTO, Masahiro	Professor
NISHI, Nobuyuki	Professor
OKAMOTO, Hiromi	Professor
NAGAYAMA, Kuniaki	Professor (OIIB)
KATO, Koichi	Professor (OIIB)
NAGASE, Shigeru	Professor
SUZUKI, Toshiyasu	Associate Professor
NAGATA, Toshi	Associate Professor
SAKURAI, Hidehiro	Associate Professor
NISHIMURA, Katsuyuki	Associate Professor
TADA, Mizuki	Associate Professor
TANAKA, Shoji	Assistant Professor
SAKAMOTO, Yoichi	Assistant Professor
HIGASHIBAYASHI, Shuhei	Assistant Professor
KAJI, Toshihiko	Assistant Professor
NAKAO, Satoru	Post-Doctoral Fellow (NanoNet project)
SUGIHARA, Takahiro	Research Fellow*
SUZUKI, Hiroko	Secretary
WATANABE, Yoko	Secretary
FUNAKI, Yumiko	Secretary
IWATA, Yumi	Secretary (NanoNet project)

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.*).

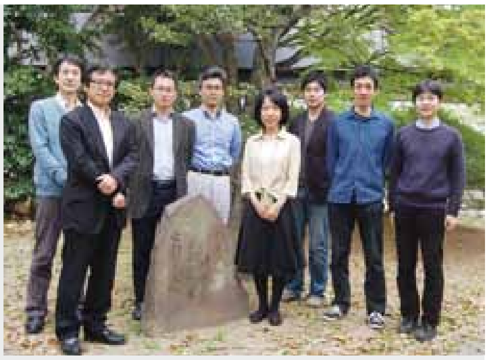
The Center also conducts the Nanotechnology Network Project of the Ministry of Education, Culture, Sports, Science and Technology (MEXT) as a core organization, and provides various kinds of nanotechnology public support programs to Japanese and foreign researchers. This project will be described in 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 JEOL

Laser Research Center for Molecular Science

OKAMOTO, Hiromi	Director, Professor
KATOH, Masahiro	Professor
OHMORI, Kenji	Professor
OHSHIMA, Yasuhiro	Professor
TAIRA, Takunori	Associate Professor
FUJI, Takao	Associate Professor
ISHIZUKI, Hideki	Assistant Professor
NOMURA, Yutaka	Assistant Professor
OKANO, Yasuaki	Technical Associate
MASUDA, Michiko	Secretary
KAWAI, Shigeko	Secretary



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.

Two of full-time associate professors and their research groups belong to the Center. The groups promote research projects targeting mainly on developments of novel laser light sources for molecular science. The Center also possesses several general-purpose instruments for laser-related measurements, and lends them to researchers in IMS who conduct laser-based studies, so as to support and contribute to their advanced researches.

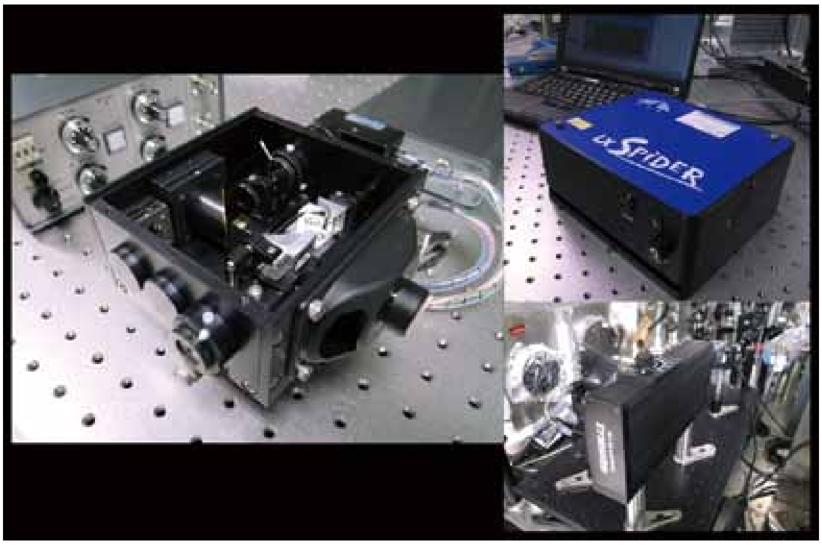


Figure 1. (left) A Fringe-Resolved Autocorrelation (FRAC) apparatus for sub-10 fs pulse characterization designed in the Center. (upper right) Spectral Phase Interferometry for Direct Electric-Field Reconstruction (SPIDER) and (lower right) Frequency-Resolved Optical Gating (FROG) apparatuses for general-purpose ultrashort pulse characterization.

Instrument Center

OHSHIMA, Yasuhiro	Director
YAMANAKA, Takaya	Technical Associate
TAKAYAMA, Takashi	Technical Associate
FUJIWARA, Motoyasu	Technical Associate
OKANO, Yoshinori	Technical Associate
MIZUKAWA, Tetsunori	Technical Associate
MAKITA, Seiji	Technical Associate
NAKANO, Michiko	Technical Associate
SAITO, Midori	Technical Associate
UEDA, Tadashi	Technical Associate
OTA, Akiyo	Secretary
NAKAGAWA, Nobuyo	Secretary

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 intend to conduct their research by utilizing general-purpose instruments. The staffs of Instrument Center maintain the best condition 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 (JEOL JNM-ECA 600, JNM-LA500, and JNM-LA400), matrix assisted laser desorption ionization (MALDI) mass spectrometer (Voyager DE-STR), powder X-ray diffractometer (Rigaku RINT-Ultima III), circular dichroism (CD) spectrometer (JASCO JW-720WI), differential scanning calorimeter (MicroCal VP-DSC), and isothermal titration calorimeter (MicroCal iTC200). In the Myodaiji campus, the following instrument are installed: Electron spin resonance (ESR) spectrometers (Bruker E680, E500, EMX Plus), superconducting quantum interference devices (SQUID; Quantum Design MPMS-7 and MPMS-XL7), powder X-ray diffractometer (MAC Science MXP3), and single-crystal X-ray diffractometers (Rigaku Mercury CCD-1, CCD-2, RAXIS IV, and 4176F07), thermal analysis instruments (TA TGA2950, DSC2920, and SDT2960), fluorescence spectro-photometer (SPEX Fluorolog2), X-ray fluorescence spectrometer (JEOL JSX-3400RII), UV-VIS-NIR spectro-photometer (Hitachi U-3500), Raman microscope (Renishaw INVIA REFLEX532), excimer/dye laser system (Lambda Physics LPX105i/LPD3002), Nd^{+}:YAG-laser pumped OPO laser (Spectra Physics GCR-250/Lambda Physics Scanmate OPPO), excimer laser (Lambda Physics Complex 110F), and picosecond tunable laser system (Spectra Physics Tsunami/Quantronix Titan/Light Conversion TOPAS). In the fiscal year of 2010, Instrument Center accepted 60 applications from 41 institutions outside IMS. Instrument Center also maintains helium liquefiers in the both campus and provides liquid helium to users. Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute. 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 Inter-University Network for Common Utilization of Research Equipments.

Figure 1. 600 MHz NMR spectrometer (JEOL JNM-ESA600).

Figure 2. Pulse ESR for Q-band (Bruker E680).

Figure 3. Raman microscope (Renishaw INVIA REFLEX532).

Equipment Development Center

KATOH, Masahiro	Director
MIZUTANI, Nobuo	Technical Associate
AOYAMA, Masaki	Technical Associate
YANO, Takayuki	Technical Associate
KONDOU, Takuhiko	Technical Associate
YOSHIDA, Hisashi	Technical Associate
UTCHIYAMA, Kouichi	Technical Associate
TOYODA, Tomonori	Technical Associate
NAGATA, Masaaki	Technical Associate
TAKADA, Noriko	Technical Associate
MIYASHITA, Harumi	Technical Fellow
SUGITO,Shouji	Technical Fellow
URANO, Hiroko	Secretary

Researches and developments 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 glass works 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.

Development of Magnetic Field Compensation Device by High Sensitive Magnetic Sensor and Helmholtz Coils

On the research of Yokoyama Group (Division of Electronic Structure), the earth magnetic field (~0.4 G) and magnetic field generated by other instruments sometimes affect the magnetic measurements and the preparation of magnetic thin films.

We have developed three axes Helmholtz coils combined with high sensitive magnetic sensor, which automatically measures the magnetic field inside an enclosed space and subsequently drives the coils to cancel the field inside. This instrument consists of 3D magnetic measurement with high accuracy, *x*,*y*,*z* Helmholtz coils, and current sources to drive the coils. The magnetic field compensation is done with a computer controlled program.

The magneto impedance (MI) sensor can measure the magnetic field up to 2 G with a resolution of 0.003 G. The constant current circuit supplies up to 2 A with a resolution of 1 mA, which is driven by the digital-to-analogue converter from PC. Through PC USB port, all the measured magnetic field is received and the coil current driving voltage is sent. The computer program keeps the magnetic field constant by a feedback control in which the controller measures the magnetic field and supplies current proportional to the deviation between the measured and target fields.

With a cage of a 30 cm cube wound with coils, we can control the magnetic field with a resolution of below ±0.005 G and with a response time of 18 ms. We are planning to improve the response time to compensate a high-speed pulse magnetic field generated by other instruments.

Figure 1. Magnetic field compensation device.

Fabrication of Multi-Wire Correction Coils for Variable Polarization Undulator in UVSOR-II

An apple-II undulator with about 3m length have been installed in UVSOR-II for producing synchrotron light of various polarization properties. However, when the undulator is operated in the vertical polarization mode, the lifetime of electron beam circulating in the storage ring significantly decreases. The reason is considered to be due to the non-linear magnetic field in the undulator, which strongly depends on the undulator gap. To cancel the non-linear field, we fabricated and installed a specially designed correction coils on the upper and the under surface of the beam duct at the undulator.

As shown Figure 2, the correction coils are made from flat copper wires each of which has a cross section of 0.3 mm × 3 mm. 14 wires have been glued onto the surface of acrylic jig which has 14 grooved lines by polyimide tapes. The wires are connected to several power supplies to produce desired non-linear field. In the test operation, it was successfully demonstrated that the lifetime of electron beam was significantly improved.

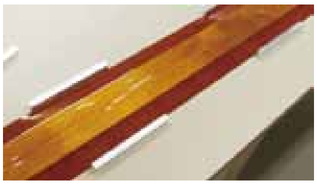


Figure 2. Correction coils.

Research Center for Computational Science

SAITO, Shinji	Director, Professor
EHARA, Masahiro	Professor
OKUMURA, Hisashi	Associate Professor
OONO, Hitoshi	Assistant Professor
ISHIDA, Tateki	Assistant Professor
KIM, Kang	Assistant Professor
FUKUDA, Ryoichi	Assistant Professor
ITOH, G. Satoru	Assistant Professor
MIZUTANI, Fumiyasu	Technical Associate
TESHIMA, Fumitsuna	Technical Associate
NAITO, Shigeki	Technical Associate
SAWA, Masataka	Technical Associate
IWAHASHI, Kensuke	Technical Associate
MATSUO, Jun-ichi	Technical Associate
NAGAYA, Takakazu	Technical Associate
TOYA, Akiko	Secretary
ISHIHARA, Mayumi	Secretary

Research Center for Computational Science provides state-of-the-art computational resources to academic researchers in molecular science and related fields, *e.g.* quantum chemistry, molecular simulations, and solid state physics. The computer systems consist of Fujitsu PRIMEQUEST, SGI Altix4700, and Hitachi SR16000. Over 660 users in 170 project groups from a wide range of molecular science have used in 2010. The large scale calculations, for example the formation of fullerenes, conformation searches using non-Boltzmann ensemble methods, and nonlinear spectroscopy of liquids, have been performed with the systems. The Center also provides a number of application programs, for example including Gaussian 09, GAMESS, Molpro, AMBER, and NAMD. The Center offers the Quantum Chemistry Literature Database, 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 113,007 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 the provision of computational resources, the Center contributes to the so-called next-generation supercomputer project which is conducted by the government. IMS and the Center play an important role in the applications of the PFlops-scale supercomputer to nano-science in Development and Application of Advanced High-Performance Supercomputer Project. Furthermore, in 2010, Computational Material Science Initiative (CMSI) was established, after the research field which consists of molecular science, solid state physics, and material science was selected as one of the research fields which scientific breakthroughs are expected by using the supercomputer. The Center contributes to CMSI by providing approximately 20% of its computational resource.

Figure 1. Super-High-Performance Molecular Simulator.

Okazaki Institute for Integrative Bioscience

AONO, Shigetoshi	Professor
KUWAJIMA, Kunihiro	Professor
KATO, Koichi	Professor
FUJII, Hiroshi	Associate Professor
KURAHASHI, Takuya	Assistant Professor
YOSHIOKA, Shiro	Assistant Professor
MAKABE, Koki	Assistant Professor
YAMAGUCHI, Takumi	Assistant Professor
KAMIYA, Yukiko	IMS Research Assistant Professor
NAKAMURA, Takashi	IMS Research Assistant Professor
SAWAI, Hitomi	IMS Research Assistant Professor
CHEN, Jin	OIIB Research Assistant Professor
TANIZAWA, Misako	Secretary
TANAKA, Kei	Secretary

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 elucidated the structure and function relationships of the heme-based sensor proteins in which a heme is the active site for sensing gas molecules such as CO and O_2. They also reported the structure and function relationships of HesR that is an heme-sensing transcriptional regulator responsible for the expression of heme efflux system. 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. In this year, they developed NMR methods for detailed conformational characterization of oligosaccharides using lanthanide tagging and stable isotope labeling. 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 equilibria and kinetics of the ATP binding to the *Escherichia coli* chaperonin GroEL. 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 monooxygenation reactions and denitification processes.

OIIB is conducting the research program, "Integrated Bioscience to Reveal the Entire Life System with Studies of Biofunctional Molecules" and "Research on the Molecular Mechanisms of Biological Responses toward Environmental- and Biological-molecules." In these research programs, the studies on the following subjects have been carried out: (i) functional analyses of higher-ordered biological phenomena, (ii) comprehensive screening of biofunctional molecules, (iii) computer simulations of higher-ordered biological systems and biofunctional molecules, (iv) molecular mechanisms of response to environmental molecules, of differentiation of germ cells, and of cellular stress-response and defense against stress, (v) studies on perturbation of biological functions induced by environmental molecules, (vi) studies on normal physiological functions regulated by biological molecules, and (vii) construction of integrated data base on the biological influences of environmental molecules.

Safety Office

TANAKA, Koji	Director
TOMURA, Masaaki	Assistant Professor
TANAKA, Shoji	Assistant Professor
SUZUI, Mitsukazu	Technical Associate
NAGATA, Masaaki	Technical Associate
YAMANAKA, Takaya	Technical Associate
UEDA, Tadashi	Technical Associate
TAKAYAMA, Takashi	Technical Associate
SAKAI, Masahiro	Technical Associate
MAKITA, Seiji	Technical Associate
ONITAKE, Naoko	Secretary
TSURUTA, Yumiko	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 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.