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 (1978–2011).

UVSOR Facility

KATOH, Masahiro	Director, Professor
SHIGEMASA, Eiji	Associate Professor
KIMURA, Shin-ichi	Associate Professor
ADACHI, Masahiro	Assistant Professor
IWAYAMA, Hiroshi	Assistant Professor
MATSUNAMI, Masaharu	Assistant Professor
OHIGASHI, Takuji	Assistant Professor
KONOMI, Taro	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

Since the first light in 1983, UVSOR has been successfully operated as one of the major synchrotron light sources in Japan. After the major upgrade of the accelerators in 2003, UVSOR was renamed to UVSOR-II and became one of the world brightest low energy synchrotron light source. In 2012, it was upgraded again and has been renamed to UVSOR-III. The brightness of the electron beam was increased further. Totally, six undulators were installed. It is operated fully in the top-up mode, in which the electron beam intensity is kept constant.

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. 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 providing SR. The bending magnet with its radius of 2.2 m provides SR with the critical energy of 425 eV. There are twelve beam-lines operational at UVSOR, two beam-lines under commissioning, one under construction. The operational beam-lines can be classified into two categories. Nine 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 other three 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. UVSOR electron storage ring and synchrotron radiation beam-lines.

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

In 2011, a new undulator system dedicated for coherent light production was constructed as shown in Figure 2. This new undulator will be used for coherent light generation both in the UV-VUV range and in the THz range. This will be also used for the resonator free electron laser.

In spring, 2012, we had three month shut-down for a reconstruction work towards UVSOR-III. We have replaced all the bending magnets in the storage ring with combined function ones which are capable of producing defocussing fields as well as the dipole fields. A new in-vacuum undulator was installed. This will be used for a scanning transmission X-ray microscope (STXM) beam-line, which is also under construction.

Figure 2. New Undulators installed in 2011. The upper is the variable polarization optical klystron undulator which will be used for coherent light generation. The lower is the in-vacuum undulator for the STXM beam-line.

Reserch Highlight 2011

A New Two-Dimensional Topological Insulator —Successful Formation of a Bilayer Bismuth

Topological insulators are a new state of matter which is gaining increased attention in condensed matter physics. While the bulk is an insulator, they have metallic edge (surface states) and these edge states have similar properties with magnets even though the bulk is not a magnet. There are hopes to develop novel devices utilizing this intriguing property.

In this work,[1)] a way to fabricate a new two-dimensional topological insulator has been found. The remarkable thing about this material is that it is only two-atomic layers (bilayer) thick made of bismuth. While it is not impossible to make such a thin material in the atomic scale (for example, the Noble physics prize in 2010 was awarded to physicists who studied graphene, a single atomic-layer sheet of carbon), it still remains to be a big challenge. The present finding should accelerate researches to further understand the exotic properties of topological insulators as well as for application in atomic-scale devices and quantum computation.

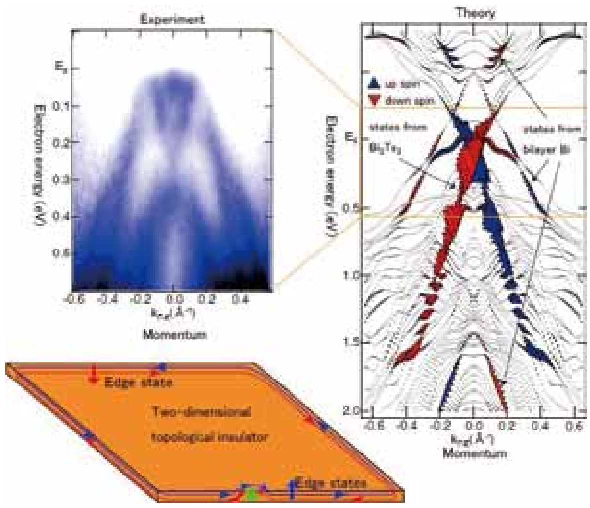


Figure 3. The experimental band dispersion of Bi(111) bilayer on Bi_2Te_3 measured experimentally (left) and its corresponding first-principles calculations (right). The left bottom figure shows the schematic drawing of a two-dimensional topological insulator.

Reference

1) T. Hirahara, G. Bihlmayer, Y. Sakamoto, M. Yamada, **H. Miyazaki**, **S. Kimura**, S. Blugel and S. Hasegawa, *Phys. Rev. Lett.* **107**, 166801 (5 pages) (2011).

Research Center for Molecular Scale Nanoscience

YOKOYAMA, Toshihiko	Director, Professor
HIRAMOTO, Masahiro	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 (Nanotechnology Platform)
KANEKO, Yasushi	Technical Fellow (Nanotechnology Platform manager)
SUZUKI, Hiroko	Secretary
WATANABE, Yoko	Secretary
FUNAKI, Yumiko	Secretary
TOYAMA, Yu	Secretary (Nanotechnology Platform)

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.

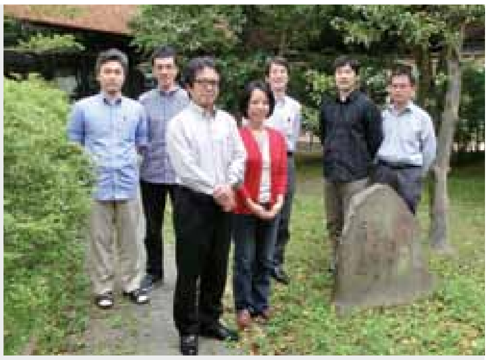
As a public research management, the Center has been conducting Nanotechnology Network Project (April 2007–March 2012) and Nanotechnology Platform Program (July 2012–March 2022) of the Ministry of Education, Culture, Sports, Science and Technology (MEXT) as a representative organization, and provided various kinds of nanotechnology public support programs to Japanese and foreign researchers. Details of these projects will be described in the other section in this book.

Through the MEXT projects, the Center 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 920MHz 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.*).

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.

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.

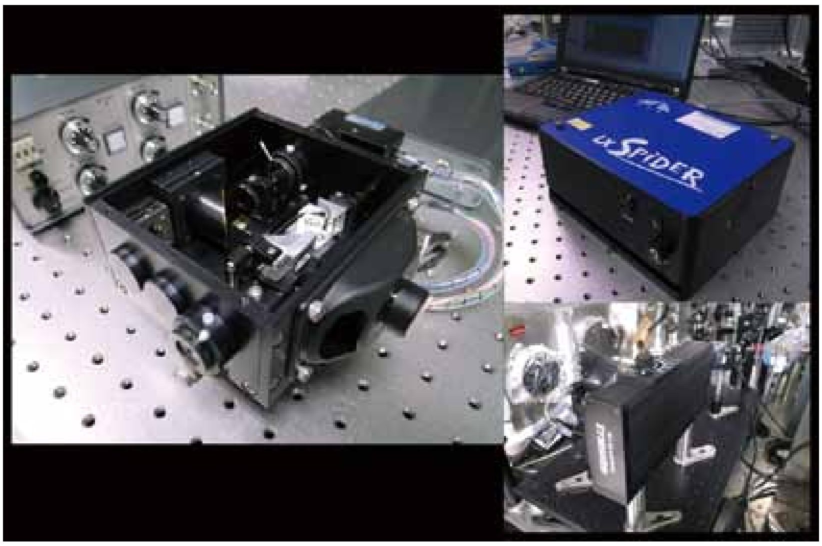


Figure 1. (left) A Fringe-Resolved Autocorrelation (FRAC) apparatus for sub-10 fs pulse characterization designed in the Center. (upper right) Spectral Phase Interferometry for Direct Electric-Field Reconstruction (SPIDER) and (lower right) Frequency-Resolved Optical Gating (FROG) apparatuses for general-purpose 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, and JNM-LA500), 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 addition to these, the following instruments have newly been added as the open facilities maintained by the Center: Electron spectrometers for chemical analysis (ESCA) (Omicron EA-125), high-resolution transmission electron microscope (TEM; JEOL JEM-3100FEF), scanning electron microscope (SEM; JEOL JEM-6700F(1), JED-2201F), focused ion beam (FIB) machine (JEOL JEM-9310FIB(P)), elemental analyzer (J-Science Lab Micro Corder JM10), NMR spectrometers (JEOL JNM-ECA920 and JNM-ECS400), and FTIR spectrometer (Bruker IFS 66v/S). In the fiscal year of 2011, Instrument Center accepted more than 80 applications from 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

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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 Seven-Axes Adjustable Stage for Manufacturing of Multi-Channel Biosensor

We are developing fine processing technologies using photo-fabrication as a new supporting technology.

We process penetrated micro-holes of about 1 to 2 µm in diameter with X-ray lithography at the specific positions on PMMA (poly-methyl-methacrylate) boards which are used for researches of biosensors, such as transferring signal of nerve cells, and so on.

We have developed a seven-axes adjustable stage for the alignment of the X-ray mask and the PMMA board accurately and conveniently. The positioning accuracy of less than 10 µm was succcessfully demonstrated.

Figure 1. Seven axes adjustable stage.

Development of Microfluidic Mixer for Research of Structural Changes in Proteins

We are developing a microfluidic mixer, which is used to investigate structural changes in proteins by mixing of two or more solutions combining with a fluorescence microscope. This is another example of the application of the photo-fabrication.

For this device, we have to produce micro-flow-channels of 10 µm width and 50 µm depth. Since it is hard to produce by ordinary machining, we have been developing techniques based on photolithography and PDMS (poly-dimethyl-siloxane) molding. We have successfully produced a microfluidic mixser as shown in Figure 2.

Figure 2. Microfluidic mixer.

BPM System Using Coaxial Switches and ARM Microcontroller through LAN

For the commissioning work after the remodeling of the UVSOR electron storage ring, which started from April 2012, we have developed a beam position monitor (BPM) system, which is capable of measuring the electron beam orbit, turn by turn. The sensor head of BPM consists of four electrodes mounted on the beam pipe. The beam position can be deduced from the difference between the induced fast electric pulse voltages on the electrodes by the beam. The electric signals are recorded by a digital oscilloscope which has four channels. The key technique of the system is switching of the BPM signals remotely from control room.

In UVSOR, there are 24 BPM heads. By using the newly developed signal switching system (Figure 3), we can select one BPM head (four signals) from 8 BPM heads. Coaxial switches of 16 SPDT types and 4 SP4T types are used. (Figure 4)

Figure 3. BPM system.

We control totally 20 coaxial switches by ‘mbed,’ the ARM microcontroller development kit. The control application is configured in a HTML file and JavaScript library, which can handle multiple I/O ports. The ‘mbed’ responds as a HTTP server when we access from LAN, and the control application is displayed on the Web browser, which enables us to select remotely the BPM signals.

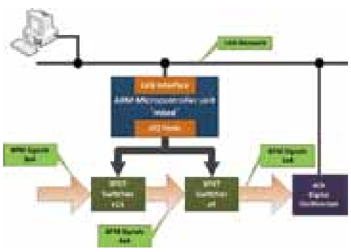

Figure 4. Block diagram of BPM system.

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
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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 PRIMERGY RX300 and PRIME HPC FX10, SGI UV1000, and Hitachi SR16000. Over 650 users, 190 project groups, in molecular science have used in 2011. 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 2008, contains 118,989 data of quantum chemical studies. Detailed information on the hardware and software at the Center is available on the web site (http://ccportal.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. 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. Fujitsu PRIMERGY RX300.

Figure 2. SGI UV1000.

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
YAMAGUCHI, Takumi	Assistant Professor
NAKAMURA, Takashi	IMS Research Assistant Professor
SAWAI, Hitomi	IMS Research Assistant Professor
CHEN, Jin	OIIB Research Assistant Professor
YAGI-UTSUMI, Maho	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 are also studying the structure and function relationships of HrtR that is an heme-sensing transcriptional regulator responsible for heme homeostasis in *Lactococcus lactis*. 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 successfully provided atomic views of conformational dynamics and intermolecular interactions of proteins involved in the ubiquitin-proteasome system and molecular recognition events on mammalian cell membranes. 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 structural fluctuations of the *Escherichia coli* chaperonin GroEL/ES complex by hydrogen/deuterium-exchange 2D NMR techniques. 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

UOZUMI, Yasuhiro	Director	
TOMURA, Masaaki	Assistant Professor	
TANAKA, Shoji	Assistant Professor	
SUZUI, Mitsukazu	Technical Associate	
NAGATA, Masaaki	Technical Associate	
UEDA, Tadashi	Technical Associate	
TAKAYAMA, Takashi	Technical Associate	
SAKAI, Masahiro	Technical Associate	
MAKITA, Seiji	Technical Associate	
KONDO, Naonori	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.