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 (1978–2009).

UVSOR Facility

KATOH, Masahiro SHIGEMASA, Eiji KIMURA, Shin-ichi ADACHI, Masahiro ZEN, Heishun IWAYAMA, Hiroshi MATSUNAMI, Masaharu HORIGOME, Toshio NAKAMURA, Eiken YAMAZAKI, Jun-ichiro HASUMOTO, Masami SAKAI, Masahiro HAYASHI, Kenji KONDO, Naonori TOKUSHI, Tetsunari HAGIWARA, Hisayo

Director, Professor Associate Professor Associate Professor Assistant Professor Assistant Professor Assistant Professor Assistant Professor Technical Associate **Technical Associate Technical Associate Technical Associate Technical Associate Technical Associate Technical Associate Technical Fellow** 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 is the extended double-bend cell 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, whose 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 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 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, 1 (far) infrared station equipped with FT interferometers.

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.



Figure 1. Overview of the UVSOR storage ring room.

Highlights of Users' Researches 2009

1) Temperature-Dependent Angle-Resolved Photoemission Spectra of EuO Ultrathin Films

H. Miyazaki, H. Mitani, T. Hajiri, T. Ito, S. Kimura (UVSOR)

Europium monoxide (EuO) is a ferromagnetic semiconductor with the Curie temperature ($T_{\rm C}$) at around 70 K. The magnetic moment originates from the half-filled 4*f* shell of the Eu²⁺ ion with a spin-only magnetic moment of S = 7/2. Recently, we reported that the origin of the magnetic properties of EuO is caused by the hybridizations of the Eu 4*f*–O 2*p* and Eu 4*f*–5*d*. Next step is to investigate the electronic and magnetic structure of thin films of a few nanometers, which is the thickness of spin filter tunnel barriers. Three dimensional angle-resolved photoemission spectroscopy (3D-ARPES) using synchrotron radiation is the most powerful technique to directly determine the electronic band structure. Using this technique we observed the change of the electronic structure across $T_{\rm C}$.

Single-crystalline EuO ultrathin films were fabricated by a molecular beam epitaxy (MBE) method. The Curie temperature $T_{\rm C}$ was about 40 K that is lower temperature than that of the bulk material. The magnetic properties and 3D-ARPES measurements were performed at the beam line 5U of UVSOR-II combined with the MBE system.

Figure 2 (a) and (b) show the energy distribution curves (EDCs) of Eu 4*f* states for EuO (100) thin films with a thickness of 100 nm and 2 nm near the Γ and X points, respectively. The band width of Eu 4*f* states of the 2 nm thickness sample become narrower compare to those of the 100 nm sample. Across the ferromagnetic phase transition, the EDC with 2 nm thickness shifts to the lower binding energy side only at the X point. The energy shifts of Eu 4*f* states with 100 and 2 nm thickness samples are 0.3 and 0.16 eV, respectively. This result indicates that the hybridization intensity between the Eu 4*f* and other states become weaker with decreasing thickness. This is consistent with the decreasing $T_{\rm C}$.



Figure 2. Temperature-dependent energy distribution curves (EDCs) of Eu 4*f* states with a thickness of 100 nm (a) and 2 nm (b) at the Γ and X point.

2) Local Environment Analysis of P Atoms in Proton-Conducting Amorphous Zirconium Phosphate Thin Films

Y. Aoki, H. Habazaki (Hokkaido Univ.)

Inorganic phosphate compounds are attractive as an unhydrated proton conductor due to the presence of large number of native acid sites. Thin film of such materials has potential as an electrolyte membrane of next-generation intermediate temperature fuel cell. Previously, we reported that amorphous zirconium phosphate thin films exhibit the enhanced proton conductivity in nonfumidified atmosphere in the intermediate temperature range. In addition, the films hydrated by heating in moisture at 400 °C exhibit the increment of conductivity by two orders of magnitude. This superior conductivity is speculated to be related to the structure of phosphate groups.

P K-edge XANES spectroscopy was carried out with *a*-ZrP_{2.5}O_x films of 40 nm, 100 nm and 300 nm-thickness (Figure 3). It is reported that P K-edge spectra of inorganic phosphate salts is very sensitive to the counter metal cation. *a*-ZrP_{2.5}O_x films show a clear peak at 2154 eV and a lower-energy, preedge peak at around 2151 eV in agreement with the spectral features of various phosphate salts. These peaks correspond to the transition from P 1s P 3p-dominant unoccupied states which satisfy the dipole selection rule. The *a*-ZrP_{2.5}O_x films possess the same features of XANES in every thickness. Furthermore, the apparent change in spectra was not observed between the as-prepared and hydrated films. These results indicate the possibility that the polymerization degree, *n*, of phosphate group P_nO_{3n+1} does not change through the hydration.



Figure 3. (a) P K-edge XANES spectra of amorphous $ZrP_{2.5}O_x$ film with thickness of (a) and (b) 40 nm, (c) and (d) 100 nm and (e) and (f) 300 nm. Solid line indicates as-prepared film and dashed line hydrated film.

Research Center for Molecular Scale Nanoscience

YOKOYAMA. Toshihiko HIRAMOTO, Masahiro NISHI, Nobuyuki OKAMOTO, Hiromi NAGAYAMÁ, Kuniaki KATO, Koichi NAGASE, Shigeru SUZUKI, Toshiyasu NAGATA, Toshi SAKURAI, Hidehiro NISHIMURA, Katsuyuki TADA, Mizuki TANAKA, Shoji SAKAMOTO, Yoichi HIGASHIBAYASHI, Shuhei KAJI, Toshihiko NAKAO, Satoru SUGIHARA, Takahiro SUZUKI, Hiroko WATANABE, Yoko FUNAKI, Yumiko IWATA, Yumi

Director, Professor Professor Professor Professor Professor (OIIB) Professor (OIIB) Professor Associate Professor Associate Professor Associate Professor Associate Professor Associate Professor Assistant Professor Assistant Professor Assistant Professor Assistant Professor Post-Doctoral Fellow (NanoNet project) **Research Fellow*** Secretary Secretary Secretary 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.*).

Since 2005, Nanoforum has been organized, which sup-

ports 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.

Laser Research Center for Molecular Science

OKAMOTO, Hiromi KATOH, Masahiro OHMORI, Kenji OHSHIMA, Yasuhiro MATSUMOTO, Yoshiyasu TAIRA, Takunori HISHIKAWA, Akiyoshi FUJI, Takao ISHIZUKI, Hideki CHIBA, Hisashi OKANO, Yasuaki MASUDA, Michiko Director, Professor Professor Professor Professor* Associate Professor Associate Professor Associate Professor Assistant Professor Technical Associate[‡] Technical Associate



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.

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Instrument Center

YAKUSHI, Kyuya YAMANAKA, Takaya TAKAYAMA, Takashi FUJIWARA, Motoyasu OKANO, Yoshinori MIZUKAWA, Tetsunori MAKITA, Seiji NAKANO, Michiko SAITO, Midori UEDA, Tadashi OTA, Akiyo NAKAGAWA, Nobuyo Director Technical Associate Secretary 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 are utilizing 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, JEOL JNM-LA400), mass spectrometer (Voyager DE-STR), powder x-ray diffractometer (Rigaku RINT-Ultima III), circular dichroic spectrometer (JASCO JW-720WI), differential scanning calorimeter (VP-DSC), and isothermal titration calorimeter (iTC200) in Yamate campus and ESR (Bruker E680, E500, EMX Plus), SQUID (Quantum Design MPMS-7, MPMS-XL7minTK), powder (MAC Science MXP3) and single-crystal diffractometers (Rigaku Mercury CCD-1 and CCD-2, RAXIS IV, 4176F07), thermal analysis instrument (TA TGA2950, DSC2920, SDT2960), fluorescence spectrophotometer (SPEX Fluorogll), x-ray fluorescence spectrometer (JEOL JSX-3400RII), UV-VIS-NIR (Hitachi U-3500) spectrophotometer, excimer+dye laser system (LPX105i+LPD3002), Nd-YAG+OPO laser (GCR-250), excimer laser (Complex 110F), and picosecond tunable laser system (TSUNAMI-TIATN-TOPAS) 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 Inter-University Network for Common Utilization of Research Equipments.

In the fiscal year of 2009 (April 2009 to March 2010), Instrument Center introduced new equipments shown below: 600 MHz NMR spectrometer for biological molecules (JEOL JNM-ESA600), pulse ESR system for Q-band (Bruker E680), Raman microscope (Renishaw INVIA REFLEX532) in Myodaiji campus. Another Raman spectrometer (JASCO NR-1800), with which low-frequency Raman is available, was transferred from Nishi group. The fluorescence spectrometer (SPEX Fluorogll) was also renewed. Instrument center is constructing original instruments collaborating with research groups inside and outside IMS. Time-resolved ESR spectrometer was constructed by Nakamura group of IMS, and calorimeter system under high-magnetic field (15 T) and very low temperature (20 mK) was constructed by Nakazawa group of Osaka University. The former is used for studying photo-excited state of organic molecules, and the latter will be used for the study of organic superconductors, organic magnets, and other materials. In the fiscal year of 2009, Instrument Center accepted 63 applications from 34 institutions outside IMS. The users mainly used SQUID (22), ESR (18), x-ray diffractometer (17), circular dichroism spectrometer (6), thermal analysis instrument (4), mass spectrometer (4), NMR (2), and Excimer-dye laser (3), where the numbers in parenthesis shows the number of use by external users.





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

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



Figure 3. Raman microscope (Renishaw INVIA REFLEX532).

Equipment Development Center

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



Design and fabrication including the research and developments of the new instruments demanded 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 researchers of other 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 Multi-Coincidence Electronic Circuit for Time-Resolved Reaction Microscopy of Electron Compton Scattering

The ultimate purpose of our project, by Prof. M. Takahashi and Dr. M. Yamazaki at Tohoku University, is to develop a new method that enables one to visualize the change of electron motion in transient species, which is the driving force in any chemical reactions. The method, time-resolved electron momentum spectroscopy (TREMS), is an experimental technique to probe vector correlations among the two outgoing electrons and fragment ion produced by Compton scattering by transient species using an ultrashort-pulsed electron beam. Here, a multidimensional coincidence electronic circuit specialized for the TREMS is required and has thus been developed in close collaboration with the IMS equipment development center.

The circuit (Figure 1) processes output signals from two position-sensitive-detectors (PSDs) of the TREMS for the electrons and ion, in the emitter coupled logic (ECL) levels. Each PSD produces seven separate output signals for each arrival of the charged particles; a time-reference signal from the microchannel plate and two delayed signals from both ends of three delay-line anodes. The function of the circuit can be divided mainly into two parts; one is AND gate logic to efficiently collect coincidence signals from the two electrons and the other is that to do so for the fragment ion associated with the electron signals. The circuit eventually produces 20 ECL logic signals (2 for time-reference signals of each PSD, 18 for delayed signals of three charged particles), only when the two electrons and ion are detected in coincidence within a certain time interval. The time sequence of the output signals is measured by a multichannel time-to-digital converter with a time resolution better than half-nanosecond. The circuit has successfully been tested using our conventional EMS apparatus; the results have completely met our expectations.



Figure 1. The multi-coincidence electronic circuit.

Micro Fabrication of Plastic Substrates for the Multichannel Incubation Type Planar Patch Clamp Biosensor

We are developing the multichannel incubation type planar

patch clamp biosensor supporting Urisu group. It is required to fabricate sub micron-level fine structures on plastic (PMMA) substrates which is the key component of the biosensor (Figure 2). As the first step, we are trying to form thin film regions with 10 µm or less thickness by hot embossing. That is, a heated metal mold is pressed against the one side surface of the plastic substrate as shown in Figure 2. At present, we have succeeded in forming about 7.8 µm-thick thin film regions with no cracks by selecting suitable thickness of plastic substrates and heating conditions. In addition, we are now developing a new both side embossing technology to fabricate micro fluidic structures on the other side surface of the plastic substrate for cell patterning. We are also developing in parallel LIGA process technology to form micro through holes with 1-2 µm diameter around at the center of the thin film region of the substrate. Here, the alignment of the through hole position, the cell soma setting area in the micro fluidic structure and the thin film region in the substrate is the most important technological problem to be solved.



Figure 2. The structure of plastic substrates for the multichannel incubation type planar patch clamp biosensor and the fabrication process.

Modification of ¹H-¹³C Double Resonance Solid State NMR Probe for 920MHz Ultra High Magnetic Field NMR

NISHIMURA group, in Department of Materials Molecular Science, is working on the new methodology and peripherals developments for solid state NMR. And we are cooperating to remodel of NMR probe.

In NMR probe, essentially, sample spinning mechanism and high voltage circuit parts for irradiation of radio frequency pulses are tightly arranged in the limited space. In this time, to realize sample temperature regulation in ¹H-¹³C double resonance solid state NMR MAS probe used in ultra high magnetic field 920MHz NMR in IMS, we have modified existing parts and also built newly designed parts. Especially, the T shape glass tube shown in Figure 3 may be worthy to mention. This is vacuum insulated double layer structure with the geometry of 14 and 12 mm outside diameter for branch and straight pipes, and 6 mm inner diameter, respectively. In order to maintain constant temperature with sample spinning at high speed, low-temperature compressed air up to 0.4 MPa is introduced from the branch pipe and a heater raised up to 400 °C is inserted into straight pipe: Therefore high insulation efficiency is required on both high and low temperature conditions. The T shape glass tube was set into the NMR probe together with other built parts (Figure 4) and the probe was tested under the supply of -40 °C compressed air, This T shape glass tube demonstrated excellent insulation efficiency and no troubles due to dew condensation has been observed. This T shape glass tube has been developed by Mr. OMARU based on his wealth of experiences and excellent techniques.

This is the first solid state NMR probe realizing sample temperature regulation on over 900MHz ultra high magnetic field NMR in Japan.



Figure 3. The T shape glass tube.



Figure 4. The T shape glass tube set into the NMR probe together with other built parts.

Research Center for Computational Science

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

Director, Professor Professor Professor Associate Professor Assistant Professor Assistant Professor Assistant Professor Assistant Professor Assistant Professor **Technical Associate 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://qcldb2.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

AONO, Shigetoshi KUWAJIMA, Kunihiro KATO, Koichi FUJII, Hiroshi KURAHASHI, Takuya YOSHIOKA, Shiro MAKABE, Koki YAMAGUCHI, Takumi KAMIYA, Yukiko NAKAMURA, Takashi SAWAI, Hitomi CHEN, Jin TANIZAWA, Misako TANAKA, Kei Professor Professor Professor Associate Professor Assistant Professor Assistant Professor Assistant Professor IMS Research Assistant Professor IMS Research Assistant Professor OIIB Research Assistant Professor Secretary 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 was the active site for sensing gas molecules such as CO and O2. They also reported the structure and function relationships of VnfA that is an iron-sulfur cluster-containing transcriptional regulator responsible for the expression of vanadium-containing nitrogenase. 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 studied the interactions between amyloid β and gangliosidic micelles and the redox-dependent domain rearrangement of protein disulfide isomerase by NMR spectroscopy in conjunction with other biophysical methods. 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 folding mechanism of β_2 -microglobulin, which is responsible for dialysis-related amyloidosis. 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 cooperation 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 TOMURA, Masaaki TANAKA, Shoji SUZUI, Mitsukazu NAGATA, Masaaki YAMANAKA, Takaya UEDA, Tadashi TAKAYAMA, Takashi SAKAI, Masahiro MAKITA, Seiji ONITAKE, Naoko TSURUTA, Yumiko Director Assistant Professor Assistant Professor Technical Associate Secretary 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.