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 (1978–2006).

UVSOR Facility

KOSUGI, Nobuhiro	Director
KATOH, Masahiro	Professor
SHIGEMASA, Eiji	Associate Professor
KIMURA, Shin-ichi	Associate Professor
HOSAKA, Masahito	Assistant Professor*
MOCHIHASHI, Akira	Assistant Professor
ITO, Takahiro	Assistant Professor
HIKOSAKA, Yasumasa	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
HAGIWARA, Hisayo	Secretary

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.

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) as well as 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. As seen in Figure 2, the numbers of users and related publications have shown an apparent upward tendency, since 2004.

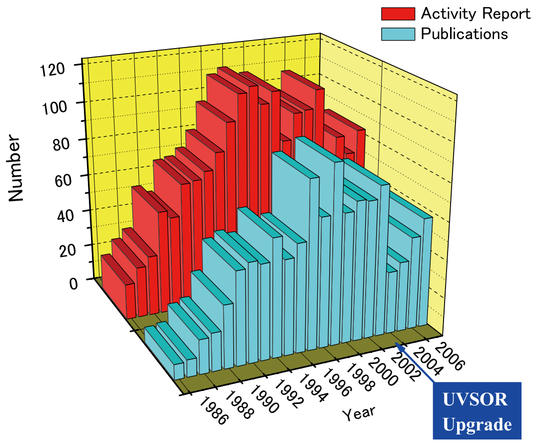


Figure 2. Number of publications resulting from UVSOR work and of users' reports in UVSOR ACTIVITY REPORT.

Highlights of Users' Researches 2006

1) VUV Reflectance Spectroscopy of Strongly Correlated Electron System

J. Fujioka, S. Miyasaka, Y. Tokura *(Univ. Tokyo, Osaka Univ.)*

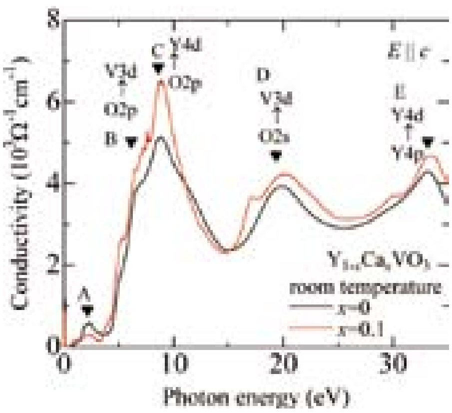


Figure 3. The optical conductivity spectra of $Y_{1-x}Ca_xVO_3$ $x = 0$ (black line) and $x = 0.1$ (red line), respectively.

The spin, orbital and charge degrees of freedom in the correlated electron system have been attracting much attention. The interplay among them leads to the versatile magnetic and/or electronic structure, even though the crystal structure is nearly cubic. The investigation of the electronic structure over wide energy range by the measurements of the reflectivity spectra is indispensable to reveal the spin-orbital-charge coupled phenomena associated with the insulator to metal transition.

We have measured the reflectivity spectra of the several transition metal oxides, including the V, Mn, Fe, Ni, and Cu ions, for an energy range between 4 eV and 35 eV. As an example, we focus on the optical conductivity spectra of the single domain crystals of the perovskite-type vanadium oxide $Y_{1-x}Ca_xVO_3$ as the prototypical Mott-Hubbard insulator, with two valence electrons in the 3*d* orbital of the nominally trivalent V ion with the spin configuration of $S = 1$.

In Figure 3, we show the optical conductivity spectra of $Y_{1-x}Ca_xVO_3$ $x = 0$ and $x = 0.10$ for $E // c$, which was measured at room temperature. We assigned the peak A around 2 eV to the Mott-gap excitation. A more intense peak (B) is observed around 7 eV, which is assigned to the charge transfer excitation from O2*p* to V3*d* level. Above 7 eV, three peaks (C, D, and E) are observed and we have assigned them to the excitations from O2*p* to Y4*d*, from O2*s* to V3*d*, and from Y4*p* to Y4*d*, respectively.

2) Phase Change of EUV Reflection Multilayer Measured by Total Electron Yields

T. Ejima, T. Harada, A. Yamazaki *(Tohoku Univ.)*

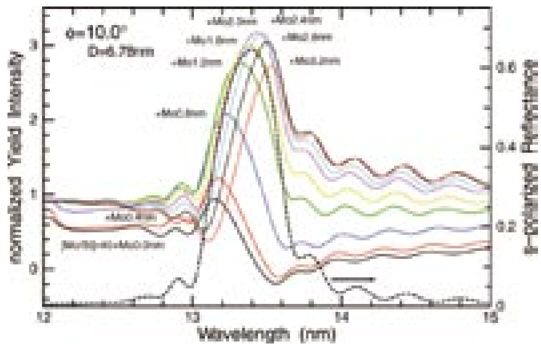


Figure 4. Total electron yield (solid curves) and reflection (broken curve) spectra of Mo/Si multilayers with varying top Mo layer thicknesses.

In the extreme ultraviolet (EUV) wavelength region, normal incidence mirrors are required to have extremely low aberrations. The surface milling method has been proposed for accurate correction of figure errors. It is essential to obtain information regarding the reflection phase in multilayer mirrors. In this study, reflection phase values for multilayer optics were obtained according to the formula derived from the total electron yield intensity and reflection in the multilayer.

Simultaneous reflection and TEY measurements for aperiodic Mo/Si multilayers are shown in Figure 4. In the TEY spectra, the main peak is observed clearly around 13.4 nm and the peak position shifts from 13.2 nm to 13.6 nm as the thickness of the top Mo layer increases. The phase term differences obtained from the reflection and TEY spectra are in accordance with the change in thickness of the top Mo layer. To evaluate the phase information, the present TEY intensity analysis has proved much easier than the Kramers-Kronig analysis of the reflection spectrum.

* Present Address; Nagoya University

Research Center for Molecular Scale Nanoscience

YOKOYAMA, Toshihiko	Director, Professor
OGAWA, Takuji	Professor
NISHI, Nobuyuki	Professor
OKAMOTO, Hiromi	Professor
NAGAYAMA, Kuniaki	Professor (OIIB)
UOZUMI, Yasuhiro	Professor
NAGASE, Shigeru	Professor
KATO, Koichi	Visiting Professor
SUZUKI, Toshiyasu	Associate Professor
NAGATA, Toshi	Associate Professor
SAKURAI, Hidehiro	Associate Professor
NISHIMURA, Katsuyuki	Associate Professor
TSUKUDA, Tatsuya	Associate Professor
TANAKA, Shoji	Assistant Professor
TANAKA, Hirofumi	Assistant Professor
SAKAMOTO, Yoichi	Assistant Professor
NAGASAWA, Takayuki	Assistant Professor
HIGASHIBAYASHI, Shuhei	Assistant Professor
SASAKAWA, Hiroaki	Assistant Professor
NOTO, Madomi	Secretary
SUZUKI, Hiroko	Secretary
WATANABE, Yoko	Secretary
ITO, Yumi	Secretary (Nanonet project)
FUNAKI, Yumiko	Sectretary (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. The research activity in the period of Sep. 2006 through Aug. 2007 was outlined as: (1) Study of folding a De Novo designed peptide, (2) Structure determination of bioactive natural products, (3) Characterization of metal ion complexes by solid state NMR, and (4) Dynamic structures of biological macromolecules. This research division 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.

Laser Research Center for Molecular Science

OHMORI, Kenji	Director, Professor
KATOH, Masahiro	Professor
OKAMOTO, Hiromi	Professor
OHSHIMA, Yasuhiro	Professor
MATSUMOTO, Yoshiyasu	Professor
TAIRA, Takunori	Associate Professor
HISHIKAWA, Akiyoshi	Associate Professor
ISHIZUKI, Hideki	Assistant Professor
WATANABE, Kazuya	Assistant Professor
UEDA, Tadashi	Technical Associate
CHIBA, Hisashi	Technical Associate
NAKAGAWA, Nobuyo	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.

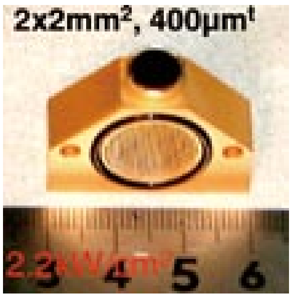


Figure 1. Microchip laser developed at the center.

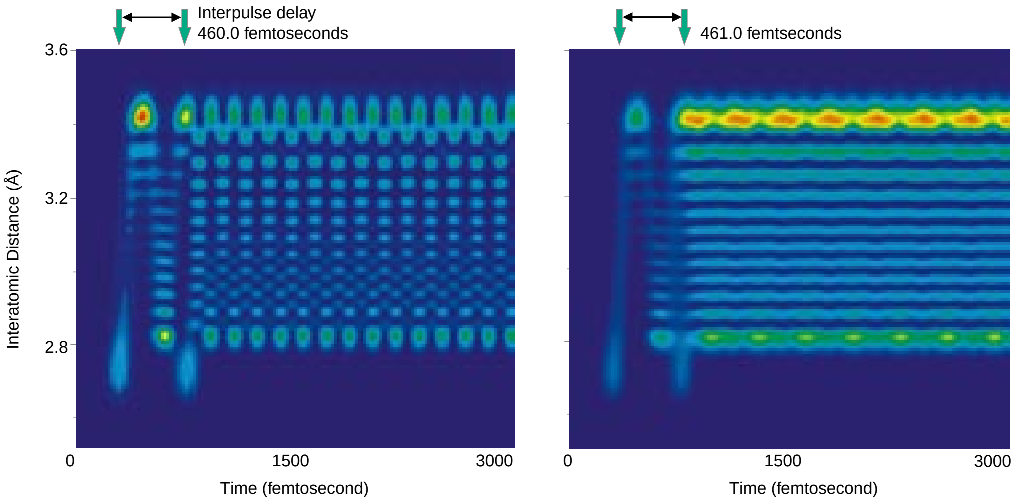


Figure 2. Theoretical simulation of quantum interferometric images generated in a single molecule with a pair of two laser pulses whose timing is controlled on the attosecond (10^{-18} sec) timescale.

Instrument Center

YAKUSHI, Kyuya	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
SAKAI, Yasuko	Secretary
OTA, Akiyo	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 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, mass spectrometer, powder x-ray diffractometer in Yamate campus and ESR, SQUID magnetometer, powder and single-crystal diffractometer, dilution refrigerator with superconducting magnet, fluorescence spectrophotometer, UV-VIS-NIR spectrophotometer, circular dichroic spectrometer 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 starts in the April of 2007. From April to July of 2007, Instrument Center accepted 17 applications from 17 institutions outside of IMS. The users applied SQUID (9), ESR (8), x-ray diffractometer (4), mass spectrometer (3), NMR (2), and UV-VIS spectrometer (1), where the numbers in parenthesis shows the application number.

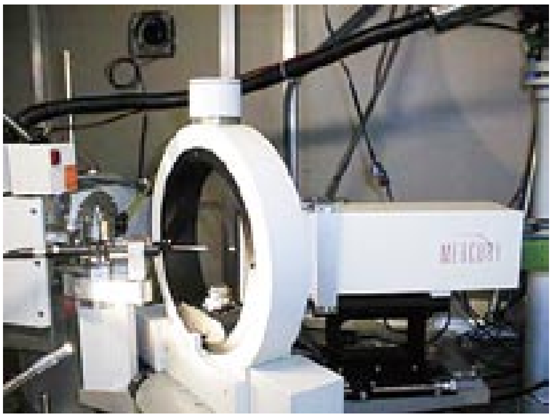


Figure 1. CCD X-ray diffractometer.

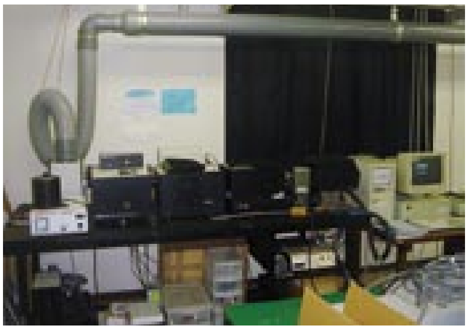


Figure 2. Fluorescence spectrophotometer.

Equipment Development Center

URISU, Tsuneo	Director
SUZUI, Mitsukazu	Technical Associate
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
MIYASHITA, Harumi	Reserch Fellow
TAKAMATSU, Yoshiteru	Reserch Fellow
URANO, Hiroko	Secretary

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.

Fabrication of a Micro Channel for a Micro Mixer

The micro mixer is a powerful apparatus that enables us to mix liquids efficiently in the micro channels as small as tens of micrometer. However, the products obtained by the mixer are sometimes contaminated by unwanted chemical reactions between the liquid and the base metal since the most of the micro mixers commercially available are made of metal. In order to prevent this, fabrication of a mixer made of a glass is required which is a technical challenge.

At the start of the project, we decided to fabricate the micro mixer by metal in order to optimize the dimensions and geometries of the micro mixer. We made micro channel of brass as shown in Figure 1 by using NC milling machine with minute end mill. The thickness of a channel wall and the distance between the channels are 100 micrometer. The channel depth is estimated to be 100 micrometer by considering the effective cutting length of an end mill used. The micro mixer we designed and fabricated consists of three parts, as shown in Figure 2.

Test experiment showed that efficiency of the mixing was not satisfactory; the results of the mixing were nearly the same with those obtained by conventional mixing. Although the reason is not clear at this moment, we believe that this is due to the fact that the wall thickness is too large. Then, we are now making an effort to reduce the wall thickness by using an end mill with a spherical shape.

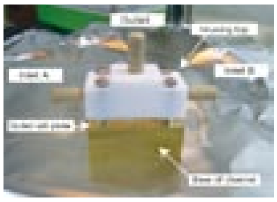


Figure 1. Micro mixer outline view.

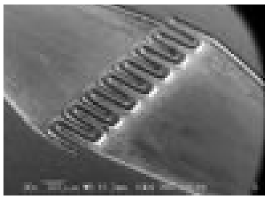


Figure 2. Micro channel.

Manufacture of the Stainless Steel Electrode Parts Using the Elliptical Vibration Cutting Method

To suppress the field emission dark current of various electron guns by high electric field sufficiently, it is required that the surface of the electrode is mirror-finish and Rz value is less than 0.1 micrometer. Titanium, molybdenum, and stainless steel are used as composition components. Currently the mirror-finish is attained by polishing. Therefore the discharge is induced by the abrasive grain remained on the surface. We applied the elliptical vibration cutting method to get a mirror-finish only by cutting those parts.

The elliptical vibration cutting method is the technique which Professor Shamoto of Nagoya University developed. The validity of this technique clarified by the ultra-precision machining using the diamond turning tool of the material, which was impossible due to the problem of a tool life until now.

Figure 3 shows photograph of the SUS304 material surface-of-a-sphere made by the elliptical vibration cutting. The best Rz value of the mirror-finished surface is 0.025 micrometer.

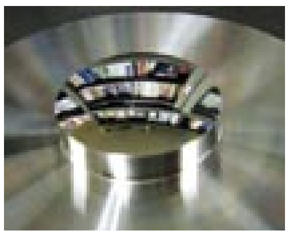


Figure 3. The 28mm diameter, surface-of-a-sphere with R60mm made by sending speed 10 micrometer/rev, spindle rotation speed 20 rpm, the vibration radius 2 micrometers and vibration frequency 39 kHz.

Research Center for Computational Science

OKAZAKI, Susumu	Director, Professor
SAITO, Shinji	Professor
MORITA, Akihiro	Professor
OONO, Hitoshi	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
YAZAKI, Toshiko	Secretary
KANO, Seiko	Secretary
TOKUSHI, Hitomi	Secretary

Research Center for Computational Sciences, Okazaki Research Facilities, National Institutes of National Science, provides up-to-date computational resources to academic researchers in molecular science and related fields. In 2006, this facility was used by 555 scientists in 141 project groups.

The computer systems, currently consisting of Fujitsu PRIMEQUEST, SGI Altix4700, NEC SX-7, and NEC TX-7, cover a wide range of computational requests in quantum chemistry, molecular simulation, chemical reaction dynamics and solid state physics. These systems are linked to international networks through Science Information Network (SINET3). Detailed information on the hardware and software of the Center is available on the web site (http://ccinfo.ims.ac.jp/).

The Center provides a number of program suites, including Gaussian 03, GAMESS, Molpro2002, Hondo2003, AMBER, 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 2006, contains 89,624 data of quantum chemical studies.

In addition to offering computer resources to wide range of 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 10TFlops. In 2006, the NAREGI project was reformed to join a new national project Development & 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	Professor
KUWAJIMA, Kunihiro	Professor
FUJII, Hiroshi	Associate Professor
KURAHASHI, Takuya	Assistant Professor
MAKI, Kosuke	Assistant Professor*
YOSHIOKA, Shiro	Assistant Professor
ISOGAI, Miho	Secretary
TANIZAWA, Misako	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.

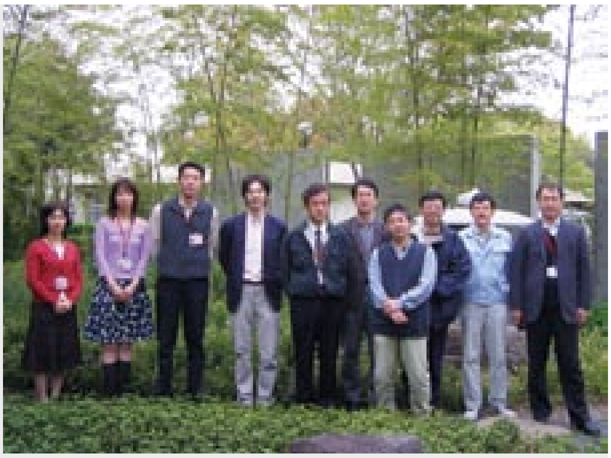
Aono group is studying the bioinorganic chemistry of hemeproteins that show a novel function. They solved the crystal structure of CO sensor protein from a thermophilic CO oxidizing bacterium and discussed the molecular mechanism of CO sensing. They also reported the structure and function relationships of aldoxime dehydratase, which is a novel heme-containing dehydrase enzyme. 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 monooxygenation 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 Electro-chemical Signaling by Membrane Proteins—Biodiversity and Principle, was held in Okazaki Conference Center from March 14 to March 16, 2007, where 19 invited lectures and 40 poster presentations were provided, and we had more than 200 participants. This symposium was co-organized as a SOKENDAI International Symposium.

* Present Address: Nagoya University, Nagoya 464-8601

Safety Office

OKAMOTO, Hiromi	Director
TOMURA, Masaaki	Assistant Professor
TANAKA, Shoji	Assistant Professor
KATO, Kiyonori	Technical Associate
HORIGOME, Toshio	Technical Associate
NAGATA, Masaaki	Technical Associate
YAMANAKA, Takaya	Technical Associate
TAKAYAMA, Takashi	Technical Associate
HAYASHI, Kenji	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.