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 (1978–2008).

UVSOR Facility

KOSUGI, Nobuhiro	Director
KATOH, Masahiro	Professor
SHIGEMASA, Eiji	Associate Professor
KIMURA, Shin-ichi	Associate Professor
HIKOSAKA, Yasumasa	Assistant Professor
ITO, Takahiro	Assistant Professor*
ADACHI, Masahiro	Assistant Professor
ZEN, Heishun	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

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 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.

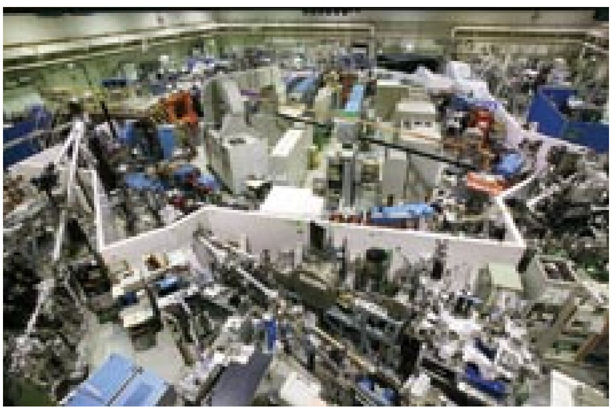

Figure 1. Overview of the UVSOR storage ring room.

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) and from enterprises (charged) are acceptable. The fruit of the research activities using SR at UVSOR is published as a UVSOR ACTIVITY REPORT annually. The refereed publications per year count more than 60 since 1996. In recent five years, the number of beamlines has been reduced from 22 to 14. The upgrade project of the UVSOR storage ring, in which the creation of four new straight sections and the achievement of much smaller emittance (27 nm-rad) were planned in 2002–2003, has been accomplished on schedule. The upgraded storage ring is named UVSOR-II. The numbers of users and related publications have shown an upward tendency, since 2004.

Highlights of Users' Researches 2008

1) Modification of Gallium Oxide Photocatalyst with Mg Ions

K. Shimura, T. Yoshida, H. Yoshida *(Nagoya Univ.)*

The development of a hydrogen production method from renewable resources and natural energy would be important to realize a sustainable society. Photocatalytic steam reforming of methane (PSRM; $CH_4 + 2H_2O \rightarrow 4H_2 + CO_2$) is an attractive reaction because it has a potential to produce hydrogen from water and biomethane by using solar energy. We applied the Ga_2O_3 photocatalyst for PSRM and examined the loading effect of Mg ions on the structure and the activity of Ga_2O_3.

Mg K-edge XANES spectrum of MgO shows some peaks and Ga L_I-edge XANES of Ga_2O_3 was broad spectrum although both absorption edges are known to appear at 1307 eV (Figure 2 (a) and (f)). The spectra of Mg^{2+}-loaded Ga_2O_3 samples calcined at various temperatures were much different from each other (Figure 2 (b)–(d)). For the sample calcined at 773 K, the spectrum was similar to that of MgO. When the calcination temperature was higher than 1073 K, the spectra were the same as that of $MgGa_2O_4$ spinel. It was suggested that Mg ions would form $MgGa_2O_4$ spinel-like local structure by substituting for Ga ions at tetrahedral site when the calcination temperature was higher than 1073 K. The Mg ions in the bulk would improve the property of the Ga_2O_3 photocatalyst.

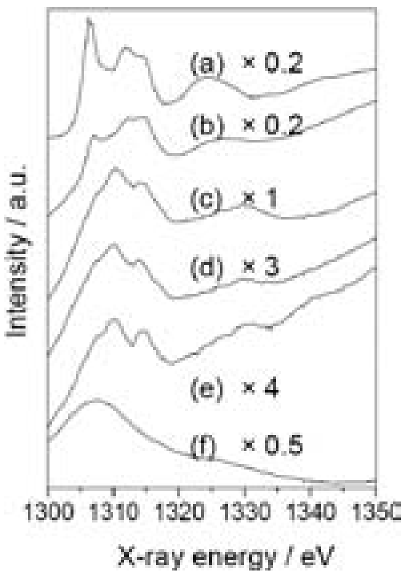

Figure 2. X-ray absorption spectra of (a) MgO, (b)–(d) Mg^{2+}-loaded Ga_2O_3 samples, (e) $MgGa_2O_4$ and (f) Ga_2O_3. Loading amount was 2 mol%. The calcination temperature was (b) 773 K, (c) 1073 K and (d) 1273 K, respectively.

2) Magneto-Optical Kerr Effect in $Nd_2(Mo_{1-x}Nb_x)_2O_7$

S. Iguchi, S. Kumakura, Y. Onose, Y. Tokura *(Univ. of Tokyo)*

The origin of the anomalous Hall effect (AHE) has long been discussed since 1960's in terms of the band effect by Karplus-Luttinger, the spin fluctuation, and the side jump, *etc*. Recent theoretical studies on the AHE due to the Berry phase or the spin-chirality mechanism are the quantum theoretical extension from the traditional perturbative treatment by Karplus-Luttinger, and have revealed the significance of the resonant effect at a small gap in band structure due to some kind of interaction, such as the spin–orbit interaction or the spin chirality. Magneto-optical Kerr effect (MOKE) is an extension of AHE with respect to the energy range. The MOKE measurements for $Nd_2Mo_2O_7$ with spin chirality and $Gd_2Mo_2O_7$ without it have revealed that there is an enhancement in the mid-IR region of the off-diagonal optical conductivity $\sigma_{xy}(\omega)$ originated from the spin chirality.

Figure 3 shows the spectra of the optical conductivity, the real and imaginary components of $\sigma_{xy}(\omega)$ in NMNO at 10 K. The $\sigma_{xx}(\omega)$ shows the correspondent change with the dc conductivity (metallic to insulating with increasing x) without remarkable anomaly such as a peak. In contrast, the characteristic peak structure was observed in the mid-IR range in the $\sigma_{xy}(\omega)$ as well as the continuity to the dc value. Especially, some of the peak-top values are larger than dc ones meaning the resonance effect is intrinsic for the off diagonal conductivity. The shift of the peak to higher energy is considered as the increase in the chemical potential by Nd doping.

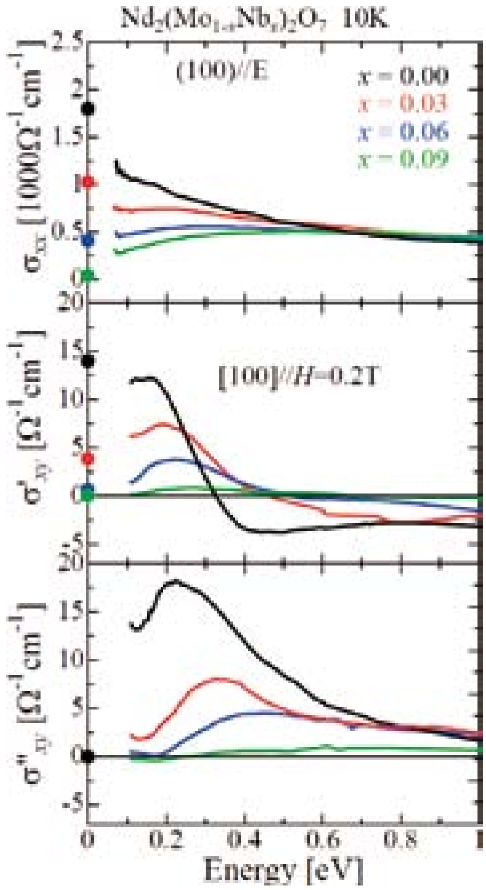

Figure 3. (a) The optical conductivity, (b) the real and (c) the imaginary part of off-diagonal optical conductivity in NMNO at 10 K.

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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)
UOZUMI, Yasuhiro	Professor
NAGASE, Shigeru	Professor
OGAWA, Takuji	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*
NOTO, Madomi	Secretary
SUZUKI, Hiroko	Secretary
WATANABE, Yoko	Secretary
FUNAKI, Yumiko	Secretary
ITO, 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*.).

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

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

* from JEOL Datum

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
CHIBA, Hisashi	Technical Associate
MASUDA, Michiko	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.

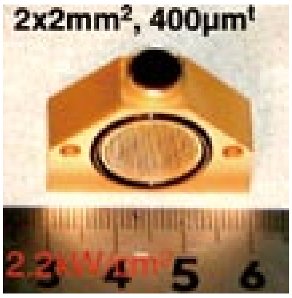

Figure 1. Microchip laser developed at the center.

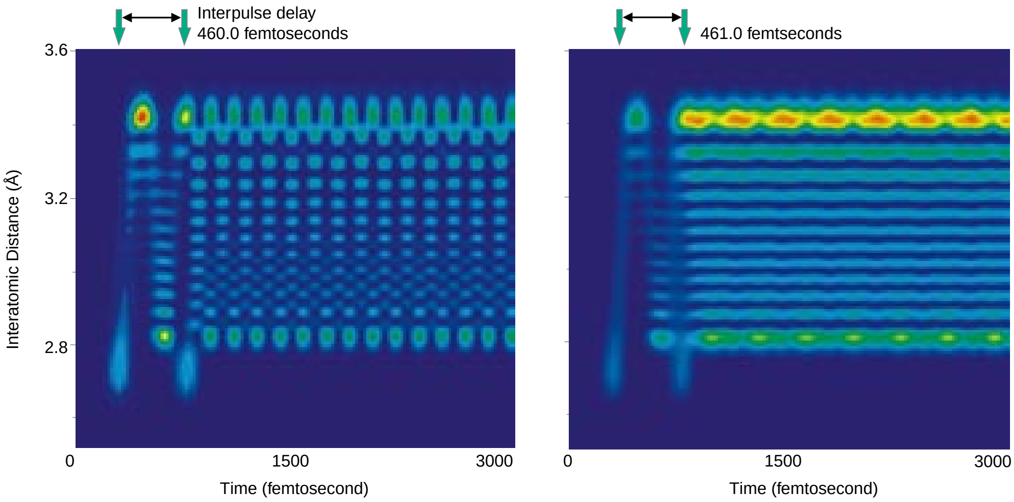

Figure 2. Theoretical simulation of quantum interferometric images generated in a single molecule with a pair of two laser pulses whose timing is controlled on the attosecond (10^{-18} sec) timescale.

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
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 are conducting their researches with the aid of 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), and circular dichroic spectrometer (JASCO JW-720WI) in Yamate campus and ESR (Bruker E680, E500, EMX Plus), SQUID (Quantum Design MPMS-7, MPMS-XL7minTK), powder (MAC Science MXP3) and single-crystal (Rigaku Mercury CCD, RAXIS IV, 4176F07) diffractometers, thermal analysis instrument (TA TGA2950, DSC2920, SDT2960), fluorescence spectrophotometer (SPEX Fluorogll), UV-VIS-NIR (Hitachi U-3500) spectrophotometer, excimer+dye laser system (LPX105i+LPD3002), Nd-YAG+OPO laser (GCR-250), and excimer laser (Complex 110F) in Myodaiji campus. Instrument Center provides liquid nitrogen and liquid helium using helium liquefiers. The staffs of Instrument Center provide consultation for how to treat liquid helium, and provide various parts necessary for low-temperature experiments. Instrument Center supports also the network sharing system of the chemistry-oriented instruments, which started in the April of 2007.

In the fiscal year of 2008 (April 2008 to March 2009), Instrument Center introduced new equipments shown below: Differential scanning calorimeter (VP-DSC) [Yamate campus], Isothermal titration calorimeter (iTC200) [Yamate campus], X-ray fluorescence spectrometer (JEOL JSX-3400RII) [Myodaiji campus]. The excimer laser of Excimer+dye laser system (Lambda physics LPX 105i + LPD3002) [Myodaiji] was renewed, and Picosecond tunable laser system (TSUNAMI-TITAN-TOPAS) [Myodaiji campus] was transferred from the research group of Professor Nishi. Instrument Center accepted 61 applications from 29 institutions outside of IMS. The users mainly used SQUID (22), ESR (20), x-ray diffractometer (24), circular dichroism spectrometer (6), thermal analysis instrument (5), mass spectrometer (4), NMR (2), and Excimer-dye laser (3), where the numbers in parenthesis shows the number of use by external users. Instrument Center provided 54,716 ℓ of liquid helium, 71,964 ℓ of liquid nitrogen, and 1,406 m^3 of nitrogen gas.

Figure 1. Differential scanning calorimeter (VP-DSC).

Figure 2. Isothermal titration calorimeter (iTC200).

Figure 3. X-ray fluorescence spectrometer (JEOL JSX-3400RII).

Figure 4. Picosecond tunable laser system (TSUNAMI-TITAN-TOPAS System).

Figure 5. Excimer+dye laser (Lambda physics LPX 105i + LPD3002)

Equipment Development Center

URISU, Tsuneo	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
TAKAMATSU, Yoshiteru	Technical Fellow
URANO, Hiroko	Secretary

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 Universal Data Logger with USB 2.0 Interface for NMR Spectroscopy

This project was proposed by Associate Prof. Kawamoto (Faculty of Science, Hokkaido University). Since FID (Free Induction Decay) signal of NMR spectroscopy decays fast and amplitude of the signal is very small, the high speed and high resolution A/D system is required. However, commercially available products are expensive and some of them are obsolete. Although USB is the most popular interface between A/D devices and computer, it is difficult to make an original interface circuit board for transmitting A/D data to a personal computer. Then, we developed the universal data logger with USB connection for high speed and high resolution A/D converter evaluation board.

We assumed the evaluation board of AD9248BCPZ-40, 14bit, dual inputs, 40MSPS A/D converter (Figure 1, left) as the target A/D device. The data from A/D converter are stored to 4Mbits SRAM controlled with CPLD XC95144XL-10TQ144 with the hardware description language, VHDL, and transmitted to computer via USB by CY7C68013A-56, high speed USB 2.0 microcontroller. The system (Figure 1, right) can be constructed with commercially available components and some customized codes.

The transfer rate of this equipment is about 13.08 msec for transmitting 4 Mbits data (4 Mbit/13.08 msec)   305.8 Mbps). This rate is sufficient for NMR Spectroscopy and most of transient measurements. Our system can be easily upgraded to up to date A/D device with minimal modifications of the source code.

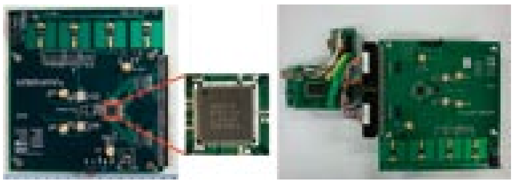

Figure 1. A/D converter and evaluation board (left) and constructed data logger (right).

Fabrication of Acrylic Substrate for 4x4 Points Type Ion Channel Biosensor

For fabrication of 4×4 points type ion channel biosensor which is currently under development in Urisu group, it is required to precisely form the 4×4 electrode inserting parts in the acrylic thin-plate (Figure 2, left). The most important point in this device is the control of thickness X in Figure 2 less than 10 µm in the acrylic substrate homogeneously at the 4×4 electrode points. In order to form this structure, we are trying hot embossing method: a heated metal mold is pressed against the acrylic substrate (cooperated by National Institute of Advanced Industrial Science and Technology (AIST)). To date, we have formed 17µm-thick thin-film in acrylic substrate. SEM image of acrylic substrate after hot embossing is shown in Figures 2 (right).

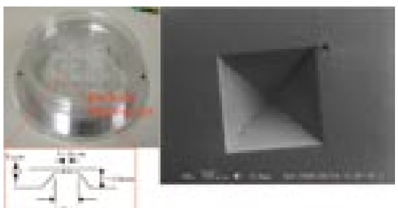

Figure 2. Multipoint type ion channel biosensor (left) and SEM image of acrylic substrate at the electrode inserting part after the hot embossing using a pyramidal mold (right).

Development of LD Pumped Passively Q-Switched Micro-Laser

We developed this equipment requested by Dr. Masaki TSUNEKANE, a member of Advanced Laser Development Division TAIRA Group, in Laser Research Center for Molecular Science. The research and study of a LD-pumped passively Q-switched micro-laser aim for laser ignition of vehicle engines taking the place of a spark plug. The developed passively Q-switched micro-laser module and a commercial spark plug are shown in Figure 3.

We have tested the various designs of micro-lasers at TAIRA Group and have improved the design for high-power, stabilization, and miniaturization. Since we achieved the energy conservation, effective ignition compared to a conventional spark plug and stable ignition for lean mixtures of gasoline and air by using the micro-laser, we have confirmed the practicality and domination of this equipment as the light source for laser ignition of engines. Now we are optimizing the design for further miniaturization comparable to a spark plug and durability to heating and vibration.

Figure 3. Compact micro-laser module.

Motorized XYZ Stages for Inverted Microscopes

This project was proposed by Prof. Urisu, who is developing an *in vitro* neural network device as a new methodology for the study of biomolecular sensing molecular science. The instrument was designed to place the PDMS stamp on the micro-pore position of the Si chip precisely (Figure 4). The specification of this stage system is shown in Table 1. It is carefully designed to provide high performance for routine applications.

Figure 4. Inverted microscope equipped on the motorized XYZ stage.

Table 1. Specification of the motorized XYZ stage.

Specifications

	PT170C-110X80Y		PA180S-200Z
	X-axis	Y-axis	Z-axis
Travel Range	110mm	80 μm	200mm
Step Resolution	1 μm	1 μm	5 μm
Position Repeatability	±1 μm	±1 μm	±1 μm
Maximum Speed	10mm/sec	10mm/sec	20mm/sec
Linear Slides	ssed roller bearings		Linear ball slide
Weight	2.4kg		17.5kg

Fabrication of a 3D Microfluidic Circuit for Compartmentalized Culture

3D micro-fluidic circuit for compartmentalized cell culture with a 25 μm hole in diameter cross-shape micro channels with 5 μm height was fabricated by injecting PDMS into a specially designed mold composing of two parts. The mold was achieved using a precise CNC milling machine, collaborating with the company supplying these molds.

Support for Outside Researchers

Table 2 shows the list of the titles which we accepted during July 2008 to June 2009. No. 1 is a design and fabrication of the apparatus to analyze the surface condition of TiO_2 photocatalyst by measuring the water contact angle without exposing to the air after cleaning of the TiO_2 surface. The photograph of the apparatus is shown in Figure 5, left. Number 5 is the fabrication of the high luminance reflection spheroid mirror. The mirror with high profile accuracy and the low surface-roughness was produced by the NC lathe followed by the hand polish processing (Figure 5, right). The number of applications to this study support from the outside researcher was about seven per year as average since 2005. More users are welcome to this system.

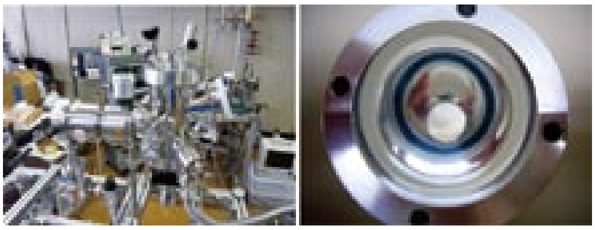

Figure 5. Apparatus for developed for the title No.1 in Table (left), and high luminance reflection spheroid mirror for No. 5.

Table 2. List of orders from outside researchers.

1	Construction of apparatus for analysis of the TiO_2 photoinduced super hydrophilicity mechanisms (HASHIMOTO, Kazuhito/The Univ. Tokyo)
2	Development of the four times reflection type X-rays telescope (TAWARA, Yuzuru/Nagoya Univ.)
3	Fabrication of the high luminance reflection mirror (BABA, Masaaki/Kyoto Univ.)
4	Development of a projection optical system and alignment stage, for ultraviolet radiation and projection exposure system (MEKARU, Harutaka/AIST)
5	Fabrication of the high luminance reflection spheroid mirror (BABA, Masaaki/Kyoto Univ.)
6	Fabrication of the Ga-compression type infrared detector (SUZUKI, Kazushi/Nagoya Univ.)
7	A compact mechanical velocity selector holder of use to analyze molecular alignment (KASAI, Toshio/Osaka Univ.)

Research Center for Computational Science

HIRATA, Fumio	Director, Professor
SAITO, Shinji	Professor
EHARA, Masahiro	Professor
OKUMURA, Hisashi	Associate Professor
OONO, Hitoshi	Assistant Professor
ISHIDA, Tateki	Assistant Professor
KIM, Kang	Assistant Professor
FUKUDA, Ryoichi	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, 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.

Award

MIZUTANI, Fumiyasu; The CSJ Award for Technical Achievements.

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
ISHIKAWA, Haruto	IMS Research Assistant Professor
KAMIYA, Yukiko	IMS 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 was the active site for sensing gas molecules such as CO and O_2. They also reported the structure and function relationships of aldoxime dehydratase, which is a novel heme-containing dehydrase enzyme. Kato group is studying structure, dynamics, and interactions of biological macromolecules primarily using ultra-high field nuclear magnetic resonance (NMR) spectroscopy. In particular, they conducted studies aimed at elucidating the dynamic structures of glycoconjugates and proteins for integrative understanding of the mechanisms underlying their biological functions. Kuwajima group is studying mechanisms of *in vitro* protein folding and mechanisms of molecular chaperone function. Their goals are to elucidate the physical principles by which a protein organizes its specific native structure from the amino acid sequence. In this year, they studied folding pathways of homologous proteins, goat α-lactalbumin and canine milk lysozyme, by experimental and computational analysis. 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, the 7th OIIB Symposium was held in Okazaki on November 12 and 13, 2008.

Safety Office

TANAKA, Koji	Director
TOMURA, Masaaki	Assistant Professor
TANAKA, Shoji	Assistant Professor
SUZUI, Mitsukazu	Technical Associate
YOSHIDA Hisashi	Technical Associate
NAGATA, Masaaki	Technical Associate
YAMANAKA, Takaya	Technical Associate
UEDA, Tadashi	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.