# RESEARCH FACILITIES

The Institute for Molecular Science includes five research facilities. This section describes their latest equipment and activities. For further information please refer to older IMS Annual Review issues (1978–2005).

## Research Center for Molecular-scale Nanoscience

This center was established in April 2002 after reorganization including the Research Center for Molecular Materials, the Department of Electronic Structure and the Department of Molecular Assemblies. The Center is supposed to play a principal role to integrate the innovative progress that IMS has achieved in the fields of molecular science and material science. Its mission is to develop a new field of science systematizing new finding in physical and chemical properties of new molecular materials and nano structures, by elucidation and controling the structure and function of the materials at the atom/molecular level. In addition, the center promote colaboration with internal and external researchers by providing technical services of common research facilities which are indispensable for nano science research.

The center is comprised of four divisions: (A) Molecular-scale electronics, (B) Nanocatalysis and biomolecular devices, (C) Nano-scale photoscience, and (D) Advanced molecular science, where the last devision consists of visiting faculty members. The respective research activities of each divisions are reported in other sections in this Review. Technical staffs are also important members of the center, who manage the common equipments and facilities of the center, provide liquid nitrogen and helium, and take care of the elemental analyses.

## UVSOR Facility

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, 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, 1 station with a multi-layer monochromator, and 1 non-monochromatized station for the irradiation of white-light.

Discussion with users, concerning the improvements and upgrades of the beamlines at UVSOR, has been continuously held as series of UVSOR workshops. 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, has been approved in the fiscal year of 2002 and has been accomplished on schedule. Keeping pace with this project, a new in-vacuum undulator and high performance monochromator for BL3U, and a new high-resolution photoelectron energy analyzer for the end station at BL5U, have been installed without any troubles. Thanks to the successful installation of the so-called magic mirror, as the first mirror of the IR beamline, BL6B, the highest intensity in the world has been achieved in the wavelength range from sub-milli to near IR region. Two vacant lots at BL2A and BL6A are available for constructing novel undulator beamlines. A new RF cavity has been installed to the short straight section between B01 and B02 before the end of March 2005; BL2A will be a bending-magnet beamline while BL6A is to be an undulator one, which will be called BL6U. From a viewpoint of radiation safety, the experiments carried out at the experimental stations on the second floor such as BL3B and BL7B, and the fine tunings of the laser system installed inside the shield walls during machine study, seem to become quite risky after introducing the so-called top-up operation of the UVSOR storage ring in the near future. Accordingly we have decided to put two old beamlines, BL8A and BL3B, out of service until the middle of March 2006. The experimental station for BL7B will be constructed at the vacant space after removing BL8A. All the beamline components have been completely removed from BL3B before the third week of March 2006. The laser system will be moved to the corresponding empty lot of BL3B by the machine group. Regarding the utilization for the long straight section between B06 and B07, a UVSOR workshop has been held in March 2005. On the basis of the review and evaluation report on the present status of UVSOR in 2004, a high resolution and high flux variable polarization beamline BL7U for spectroscopy in the VUV range has been proposed. The construction of the new beamline BL7U has begun in summer 2006, and the beamline commissioning will be started after the installation of a new variable polarization

undulator at the end of October 2006. Further discussion toward utilizing the available straight sections most effectively and formulating a basic plan on the beamline construction, will be continued.

All users are required to refer to the beam-line manuals and the UVSOR guidebook (latest revision in 1999), on the occasion of conducting actual experimental procedures. Those wishing to use the open and in-house beamlines are recommended to contact with the stationmaster/supervisor and the representative, respectively. For updated information of UVSOR, http://www.uvsor.ims.ac.jp/.

### Laser Research Center for Molecular Science

This center was established in 1997 by reorganization of a part of the Instrument Center. The Center is aimed at developing new lasers suitable for pioneering researches in the new field of molecular science and now plays a central role in promoting the special research project on "Extreme Photonics."

In addition to promoting researches, this Center maintains laser systems and supplies them to other community members. The laser systems are excimer lasers and solid-state light sources in various temporal and spectral regions, including femtosecond optical parametric oscillators (OPO), and the synchronously pumped femtosecond (OPO) (OPAL; Spectra Physics) tunable from 1.1 μm up to 1.6 μm. The Center also has general instruments and spectrophotometers, including a fluorescence spectrophotometer (Fluorolog II; Spex) composed of a xenon lamp house for excitation, double and single monochromators for spectroscopy, and changeable detectors (CCD and photomultiplier tube), UV-VIS and IR spectrophotometers, circular dichroism dispersion photometer, and general-purpose electronic instruments. Using these instruments, researchers can carry out various experiments not only in the ultrafast temporal region but also in the steady state regime.

### Equipment Development Center

R & D of the new instruments necessary for the molecular science research including the conventional services for the design and fabrication of the instruments, are the mission of this center, which consists of the mechanical, electronic and glass work sections.

We expanded our service to researchers in other universities and research institutes since 2005. The main aim of this new attempt is to improve the technology level of the center staffs, together with contributing to the molecular science community.

In this fiscal year, the total number of the services based on this new program were 14, and we consider that the original aim of this new service was filled both in quality and quantity.

*Design and fabrication works of this fiscal year*

Diebonding system for laser crystal
Electrode assembly for the threshold electron-photoion coincidence spectrometer
Poling instrument
Flexure stage
Mounting bracket for ESR cryostat
Gas nozzle and optical port for photoelectron spectrometer
Measurement chamber of biosensor
Reflection chamber
Measurement chamber of patch-clamp
Experimental compact laser module
Measurement chamber of single ion channel recording
Electron yield detector with adjustment of *Z*-axis

*Research and developments of the new instruments*

Manufacture of a mold for a microchip using a surface impression agent
A compact mechanical velocity selector to analyze molecular alignment
Activities are described in detail in the section "RESEARCH ACTIVITIES"

### Safety Office

The Safety Office was established in April 2004. The Office is supposed 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 and health office personnel, operational chiefs, and other staff members appointed by the Director General.

## Okazaki Research Facilities (related to IMS)
## Research Center for Computational Science

The 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. As of March 2006, this facility is used by 520 scientists in 132 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 Super Science Information Network (super SINET). 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 Release 2005, contains 82,017 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 participated 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 & 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://nanogc.ims.ac.jp/nanogc/).