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 (1978–2003).

Laser Research Center for Molecular Science

This center was established in 1997 by reorganization of a part of the Instrument Center. The new Center is composed of three research groups which are asked to develop new lasers suitable for pioneering researches in the new field of molecular science. The three groups are

1. Advanced Lasers for Chemical Reaction Studies,
2. Advanced Lasers for Synchrotron Radiation Applications, and
3. Advanced UV and IR Tunable Lasers.

The Laser Research Center is equipped with excimer lasers and solid-state light sources in various temporal and spectral regions, including femtosecond optical parametric oscillators (OPO). The synchronously pumped femtosecond (OPO) (OPAL; Spectra Physics) is tunable from 1.1 μm up to 1.6 μm.

The Laser Center also has general instruments and spectrophotometers. A fluorescence spectrophotometer (Fluorolog II; Spex) is composed of a xenon lamp house for excitation, double and single monochromators for spectroscopy, and changeable detectors (CCD and photomultiplier tube). Other instruments are 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.

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, (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.

Equipment Development Center

Design and fabrication of the instruments, and research and developments of the new instruments necessary for the molecular science research are the mission of this center, which consists of the mechanical, electronic and glass work sections.

Design and fabrication works of this fiscal year

Head of microchip Yb:YAG laser
Diebonding system
Water manifold for LD
Lens holder in diode-pump module
Improvement of diebonding system for laser crystal
Accurate diebonding system using SiC heater
Laser cooling system
Micro-laser and holder
Double stage acceleration time-of-flight mass spectrometer
Auger yield detection system
Micro-manipulator

Research and developments of the new instruments

High-Precision slit
Beam positioning system

Activities are described in detail in the section “RESEARCH ACTIVITIES.”

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 about 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 300 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 16 beamlines operational at UVSOR, which can be classified into two categories. 8 of them are 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 8 beamlines are 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 3 non-monochromatized stations for irradiation of white-light.

The replacement of the old planar undulator into an in-vacuum type one with 2-m long has been successfully accomplished in 2003. The length of the undulator period and the number of the periods are 38 mm and 50, respectively. This new undulator covers the spectral region from 50 to 120 eV with its first harmonic radiation. The carbon, nitrogen, and oxygen K-edge regions, which are main targets on the novel in-house beamline BL3U, can be covered with the use of the third and fifth harmonics. The helical undulator was installed in 1996, which can also be used as the helical optical klystron for free electron laser (FEL) experiments. The undulator supplies the perfect circular polarization in the photon energy range of 2–45 eV, and the elliptic polarization up to 200 eV.

Discussion with users, concerning the improvements and upgrades of the beamlines at UVSOR, has been continuously made as series of UVSOR workshops. Discussion for the rebuilt and rearrangement of several old beamlines has been initiated more recently, on the basis of the review and evaluation report on the present status of UVSOR in 2000. According to the decision through the discussion, the reconstruction of BL3U and BL6, and the introduction of high-resolution photoelectron spectrometer to BL5U have begun in 2002. The upgrade project of the storage ring, which is intended to realize much smaller emittance (27nm-rad) and create new straight sections, was funded in FY2002 and the construction of accelerator components, beamlines, and the spectrometer has begun in 2002. All the reconstruction work has been completed by the end of July in 2003, and then the commissioning of the upgraded UVSOR, UVSOR-II, has started. The operation of UVSOR-II for users has been started successfully from the first week of September 2003, and so far there has been no serious trouble on the machine operation of UVSOR-II.

All users are required to refer to the beam-line manuals and the UVSOR guidebook (latest revision in 1999), on the occasion of conducting the 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/.

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 Faciities (related to IMS)
Research Center for Computational Science

Research Center for Computational Science, Okazaki Research Facilities, National Institutes of Natural Sciences, provides up-to-date computational resources to academic researchers in molecular science and related fields. As of March 2004, this facility is used by 550 scientists in 133 project groups.

The computer systems, currently consisting of Fujitsu VPP5000, SGI 2800/Origin3800, NEC SX-7, NEC TX-7 and Hitachi SR8000, 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, Hondo2002, 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 2004, contains 68,468 data of quantum chemical studies.

In addition to offering computer resources to a wide range of molecular scientists, another vital aspect of the Center is to perform leading computational researches with massive computations. Since 2003 the Center is participating in the National Research Grid Initiative (NAREGI) project, a five-year national project by National Institute of Informatics (NII) and IMS. This joint project aims 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. Further information on the NAREGI project and the computer systems at the Center is found on the web site (http://nanogrid.ims.ac.jp/nanogrid/).