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 (1978–2002).

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 materials science. Its mission is to develop a new frontier of science that aims at constructing novel nanometer-scale materials, and elucidating the behavior thereof, on the basis of understanding the structure and dynamics of each molecular component.

The scientific research in this Center is carried out in the five laboratories: (A) Molecular-scale Electronics, (B) Nanocatalysis and Biomolecular Devices, (C) Nano-scale Photoscience, (D) Interface Molecular Science, and (E) Molecular Clusters, where the latter two laboratories consist of the faculty members transferred from other universities. The respective research activities of these laboratories are reported in the other sections in this Review. The Center also contains the supporting facilities, which manage the instruments (EPR, SQUID, NMR, *etc.*) for inter-university use, provide liquid N_2 and He for research and machine maintenance, and take care of the elemental analyses and the mass spectrometric measurements of chemical materials.

Equipment Development Center

A number of research instruments have been designed and constructed at the mechanical, electronic and glasswork sections in this Facility. Examples of our works in this fiscal year are listed below.

400MHz Gain-of-10 High-speed Signal Amplifier
Internet Compatible Remote Data Acquisition System
Multi-channel Micro-ampere Constant Current Source
Fast Rising High-voltage Pulse Generator
Interlock Circuit for Vacuum Chambers.
Thin-window X-ray cell
Quartz Cell
Microphone cell
Conections for crystals cooling system
Diodelaser focusing line
Two-stage vacuum chamber for precise alignment of the visible laser with extreme
UV light beam
Z axis stage used in scannig near-field optical microscope
Double stage acceleration time-of-flight mass spectrometer
A mount for corner-cube prism chain
A magnetic coil mount for trapping of He atoms
Insertion device for 28T Hybrid MagnetSample holder
Buffer chamber

Development of Special Machine

Equipment Development Center is also engaged in developing Special Machine. This activity is described in

detail in section “RESEARCH ACTIVITIES.”

Ultraviolet Synchrotron Orbital Radiation 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 350 mA and 70 mA, respectively.

The upgrade project, 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 has begun in 2002. All the quadrupole and sextupole magnets installed previously have been replaced with combined function magnets, which can generate both quadrupole and sextupole fields. Sixteen vertical steers that is almost twice as large in number than before, have been installed. All the power supplies for the storage ring magnets and their control system, all the beam ducts at the quadrupoles and sextupoles, three of the beam ducts at the bending magnets, the electron-gun for the injection linac and its power supplies, and the pulse modulator of the klystron have been replaced. By the end of March 2003, the fabrications of all these components were completed and their installation was initiated in April 2003, which was a month behind schedule due to the vacuum accident in November 2002 as described below.

Eight bending magnets and two 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 will be a total of 18 beamlines operational at UVSOR, which can be classified into two categories. 9 of them are so-called “Open beamlines,” that 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 9 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, 8 EUV and SX stations with a grazing incidence monochromator, 4 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 Spring 2003. The length of the undulator period and the number of the periods are 38 mm and 50, respectively. This new undulator will cover 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, will 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. In order to demonstrate the capability of FEL, the combination experiments of the non-monochromatized undulator radiation at BL3A1 with FEL have been continued last year. Further development related to the practical usability of FEL is in the planning stage.

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.

In 13th November 2002, a vacuum leakage happened. The origin of the leakage was a beam shutter at the front-end of BL1B, whose cooling water came into the ultra-high vacuum (UHV) system through a pinhole between the water channel and the surface of the shutter in UHV. The water vapor spread immediately inside the whole UHV ducts of the storage ring, and many components of the UHV system of the storage ring have been seriously damaged. As a result, the users’ beamtime for approximately a month has been canceled. The great effort by the UVSOR staff, especially the machine group, has led to quick recovery from such a serious accident, and enabled the operation of the ring to be restarted in the middle of December 2002. Finally, the user time was resumed on 24th December 2002 and was terminated by the end of March 2003. All the reconstruction work as mentioned above has been completed by the end of July, and the commissioning of the upgraded UVSOR, UVSOR-II, has begun in July 2003. The alignment of the optical elements at each beamline using visible light is under progress.

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/.

Computer Center

Since April, 2000, Computer Center of IMS has been reorganized as Research Center for Computational Science in Okazaki National Research Institute. The main super-computers at the Center consist of a vector parallel system

of Fujitsu VPP5000 and a scalar parallel system of SGI 2800. The VPP5000 system has 30 vector CPU-nodes and 256 GB of main memory. The SGI system has 320 CPUs and 320 GB of memory. NEC SX-7 and NEC TX-7 are also installed for general-purpose computations. These computers are linked to international networks through Science Information Network (SINET).

We have two types of application categories: (a) Use-of-Facility Program is open to all the domestic scientists in molecular science and related fields; (b) Advanced Research Project is for large-scale computational projects which require resources in excess of the limit for (a) Use-of-Facility Program. The projects applying for the category (b) must be expected scientifically significant achievements. About 20% of the CPU time is used by research staffs in the Institute, while the remaining 80% is given out as research grants described above to outside scientists. As of March 2003, the number of project groups was 191 with 587 users. Some of the famous package programs in Molecular Orbital Theory, *e.g.* Gaussian98, Molpro2000, Hondo, *etc.*, are kept updated as Library Programs for immediate use on the super-computers of the Center. The information for each program can be found on our Web page (http://ccinfo.ims.ac.jp/).

The Quantum Chemistry Literature Database (QCLDB) has been developed by the Quantum Chemistry Database Group in collaboration with staff members of the Center. The latest release, QCLDB Release 2002, contains 57,037 data. This database is accessible through the Web page (http://qcldb.ims.ac.jp/).