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 (1978–2000).

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 are equipped with excimer lasers and all-solid-state light sources in various temporaland spectral regions, including femtosecond and nanosecond Optical Parametric Oscillators (OPO). The synchronously femtosecond OPO (OPAL; SPECTRA PHYSICS) is tunable from 1.1 µm up to 1.6 µm. The nanosecond OPO has extraordinarily wide tuning range form 420 nm down to 2.2 mm. The Laser Center also has a fluorescence analyzer (FLUOROLOG2; SPEX) which is composed of a xenon lamp house, and double and single monochromators for spectroscopy. The detector is changeable by rotating a mirror (CCD and PM). Using these instruments, one can carry out various experiments not only in the ultrafast temporal region but also in the steady-state photon-counting region.

Research Center for Molecular Materials

The center was established by reorganization of Chemical Materials Center, Low-Temperature Center, and a part of Instrument Center in 1997. This center plays important roles in the preparation of novel chemical materials, management of chemicals in the institute, and support of liq. N_2 and He. Four research groups in the center cover the following four general research fields. 1) Preparation of Novel Heterocyclic Compounds and their Molecular Assemblies. 2) Electronic Structures and Reactivities of Metalloproteins. 3) Molecular Design of Artificial Photosynthesis System. 4) Organic Molecular Materials with Novel Electronic Properties. In addition to the research activities, the center supports the instruments including high filed NMR, EPR and MALDI-TOF mass spectrometers, SQUID, X-ray diffractometers. The center accepts the elemental analyses and mass spectrometric measurements.

Equipment Development Center

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

Ion stack
Ion beam bender
Ion(Einzel) lens
Supporter for the quadruple mass filter
Interlock circuit of UVSOR BL4B beamline
High precision dual delayed gate pulser
High speed valve controller for molecular beam source
30KV Fast rising pulse generator
Data acqusition system for Acousto-Optical spectrometer
Vacuum gauge for halogen gas

Development of IMS Machines

Equipment Development Center is also engaged in developing IMS Machines. 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 user beam time, and the lifetime of the electron beam has been improved to about 5 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 three weeks a year, which provides pulsed synchrotron radiation (SR) for time-resolved experiments. Typical beam currents under multi-bunch and single-bunch modes are 200 mA and 50 mA, respectively. Construction of a new beam position monitoring system and an orbit feedback system was completed by the end of March 2001.

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. There is a total of 20 beamlines operational at

UVSOR, which are classified into two categories. 11 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 9 beamlines are so-called “In-house beamlines,” which are dedicated to the use of the research groups within IMS. We have two soft X-rays (SX) stations each equipped with a double-crystal monochromator, eight EUV and SX stations with a grazing incidence monochromator, four VUV stations with a normal incidence monochromator, one (far) infrared station equipped with FT interferometers, one station with a multi-layer monochromator, and four non-monochromatized stations for irradiation of white-light.

The planar undulator is composed of 24 pairs of permanent magnets, the period of which is 84 mm. The fundamentals from the undulator provide quasi-monochromatic intense radiation in the photon energy region from 8 to 52 eV. 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. It was finally decided in 2000 that the superconducting wiggler for BL7A, which has a fatal problem on its cryogenic system, would be removed from the storage ring. An in-vacuum type undulator will be installed at the straight section, after removing the wiggler, in March 2002. Recently, a combination of the non-monochromatized undulator radiation at BL3A1 with FEL has led us to the success of realizing two-photon experiments for Xe atoms. To our knowledge, this is the first result indicating the practical usability of FEL in the whole world.

Discussion with users, concerning the improvements and upgrades of the beamlines at UVSOR, has been continuously made as series of UVSOR workshops. As a result, about one third of beamlines have been upgraded in recent years. BL 6B, which was originally constructed for IR experiments, is under renewal for nano-scale photochemical reaction experiments. A new high-resolution beamline BL4B in the SX region has been successfully constructed lately and its performance tests have been terminated at the end of January 2001. Several novel results for simple molecules have emerged from this beamline, using photoabsorption and angle-resolved photoion yield spectroscopy under high-resolution condition. More recently, discussion for the rebuilt and rearrangement of several old beamlines has been initiated, on the basis of the review and evaluation report on the present status of UVSOR in 2000.

In spring 2001, we had one-month shutdown to perform periodic maintenance for the rings and beamlines and to check the incidental facilities in UVSOR. During the regular shutdown period for about one month in summer 2001, similar maintenance is under progress. There were lots of trouble in one year (from September 2000 to August 2001) due mainly to the superannuated laboratory equipment, as usual, but fortunately, they did not seriously affect the user’s beam time. It should be noted that the incident of the leakage of toxic BF_3 gas happened at BL3A2 on the 22nd of December 2000. It was fortunate that nobody’s health was damaged by this accident due to a small amount of the leakage gas. A new safety system for the handling of toxic gas has been introduced to prevent further undesirable accidents.

All uses 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 1 of 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 the vector parallel system of Fujitsu VPP5000 and the scalar parallel system of SGI 2800. The VPP5000 system has 30 vector CPU-nodes, and has 256 GB of main memory. SGI 2800 has 256 CPU and 256 GB of memory. The NEC SX-5 and the IBM SP2 parallel computers are also installed for the general purpose computations. These vector and parallel computers are actively utilized mainly for the large scale molecular science simulations. The computers are linked to international networks through Science Information Network(SINET). About 25% of the computer time is dedicated by the research staff at IMS. The remaining 75% is given out as research grants to scientists outside the institute in molecular science and related field, e.g. bioscience, bioinfomatics. As of March 2001, the number of project group was 162, consisting of 643 users. The library programs of the Center amount to 807. Among them, more than 150 programs can be executed immediately. Information on the library program can be found on our center’s home-page (http://ccinfo.ims.ac.jp/). The Quantum Chemistry Literature Database (QCLDB) has also been developed by the QCLDB group in collaboration with the staff member of computer center, and this database can be accessible through our home page.