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 (1978–2001).

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 temporal and 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 from 420 nm up to 2.2 μm. 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-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 (based on quantum chemistry and statistical mechanics) and materials science (design and synthesis of functional molecules). 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 facility, which manages the instruments (EPR, SQUID, NMR, *etc.*) for inter-university use, provides liquid N_2 and He for research and machine maintenance, and takes 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 glass work sections in this Facility. Examples of our works in this fiscal year are listed below.

Specially designed insert for cryogen-free superconducting magnet
Hi precision angle resolved NMR probe
FTIR sample holder and sample exchange stage
Equipment for production of fullerenes
VUV light separation box
Electron yield detector with adjustment of Z-axis
Multi-channel Micro-ampere Constant Current Source
Bipolar High Voltage Pulse Generator
Ultra-Fast Rising Avalanche Transistor Switching Circuit
High Speed Valve Controller for Molecular Beam Source
Current-to-Voltage Converter for STM
Thin-window X-ray cell
Quartz cell

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 a 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. In order to realize much smaller emittance (27 nm-rad) and create new straight sections, a new lattice for the UVSOR storage ring was designed. This upgrade project has been approved in 2002 and preparation towards the actual reconstruction for the storage ring, which includes the replacement of all the quadrupole and sextupole magnets, has begun in spring 2002. A new position monitoring system for the photon beam was smoothly installed by the end of August 2002.

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 one soft X-rays (SX) station 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. This undulator will be replaced with an in-vacuum type undulator in March 2003. 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. An in-vacuum type undulator was successfully installed at the straight section between B06 and B07, after removing the wiggler, in March 2002. A combination of the non-monochromatized undulator radiation at BL3A1 with FEL led us to the success of realizing two-photon experiments for Xe atoms last year. Further development related to the practical usability of FEL is in progress.

Discussion with users, concerning the improvements and upgrades of the beamlines at UVSOR, has been continuously made as series of UVSOR workshops. Several novel results have emerged from the beamlines that have just been constructed. 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. It has been settled that the reconstruction of BL3 has been given the highest priority after the upgrade of the UVSOR storage ring. The reconstruction of BL6 and introduction of high-resolution photoelectron spectrometer to BL5A have also been decided through the discussion.

In spring 2002, we had a 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 approximately one month in summer 2002, similar maintenance is under progress. There were a lot of trouble in one year (from September 2001 to August 2002) due mainly to the superannuated laboratory equipment, as usual, but fortunately, they did not seriously affect the user's beam time.

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, 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 256GB of main memory. The SGI system has 320 CPUs and 320GB of memory. NEC SX-5 and IBM SP2 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 27% of the CPU time is used by research staffs in the Institute, while the remaining 73% is given out as research grants described above to outside scientists. As of March 2002, the number of project groups was 148 with 605 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 2001, contains 57,037 data. This database is accessible through the Web page (http://qcldb.ims.ac.jp/).