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 (1978–1999).

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 profitable 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.

Pulsed discharge nozzle attachment
Clamp-type diamond anvil high pressure cell
NMR probe for anisotropic measurements
New scaler system for sine bar mechanisms of UVSOR BL7B beamline
Polyethylene lens for millimeter wave spectroscopy
Data processing program for thermoelectric power measurement
TE module temperature controller
High speed valve controller for molecular beam source
Multichannel microampere constant current source
The surface profiler for optical elements
Thin cell for X-ray
Vacuum line apparatus
Quartz cell

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. A harmonic cavity was commissioned in spring 1993 to suppress longitudinal coupled-bunch instability by Landau damping. The double RF system is routinely operated for user beam time, and the lifetime of the beam has been improved to about 5 hours at 200 mA. The storage ring was divided into four sections by gate valves in spring 1995 in order to make a scheduled shutdown easier. The baking system was also replaced by new one including a controllable indirect heating. The RF power amplifier systems of the booster synchrotron and the storage ring were renewed to solid-state systems in 1996 in order to have more stable operation and easier maintenance. The storage ring is normally operated under multi-bunch mode with partial filling. The single bunch operation is also conducted about three weeks in a year to provide pulsive SR for time-resolved experiments. A resonance transverse kicker was installed in spring 1997 to keep the bunch purity and to study phase dynamics. Typical beam currents under multi-bunch and single-bunch modes are 200 mA and 50 mA, respectively.

The UVSOR storage ring consists of eight bending magnets and three insertion devices. The bending magnet having 2.2 m in radius provides the synchrotron radiation, the critical energy of which is 425 eV. The superconducting wiggler is a wavelength shifter type. The 4T magnetic field can provide soft x-rays up to 6 KeV. A planar undulator consists of 24 pairs of permanent magnets, a period of which is 84 mm. The fundamentals from the undulator provide quasi-monochromatic intense radiation in the range from 8 to 52 eV. A helical undulator was installed to one of the four straight sections of the storage ring in 1996. An optional version of the helical undulator is a helical optical klystron, which is powerful for a free electron laser experiment. The helical undulator consists of two sets of permanent magnets producing a vertical magnetic field and four sets of permanent magnets making a horizontal magnetic field. The four sets of magnets can move in the transverse direction to switch the helicity of the circular polarization. The helical undulator can provide the perfectly circular polarization in the range of 2–45 eV, and the elliptic polarization up to 200 eV. Unfortunately, the superconducting wiggler was shutdown at the beginning of June in 1999 due to the serious problem of the cryogenic system.

Initially 15 beam lines were constructed giving priority for the study of the four fields; “Spectroscopy,” “Photoelectron spectroscopy,” “Photochemical reaction,” and “Elementary process of chemical reaction.” Several years later, 4 beam lines were added to expand the research to the fields, “Solid and surface photochemical reaction” and “Photochemical material processing.” In recent years, “Combination of synchrotron radiation with laser beam” was proposed to add in the important research fields.

The UVSOR have discussed the improvements and upgrades of the beam lines with users. The workshops concerning on VUV beam lines for solid-state research, beam lines for soft x-ray, chemical reaction, and gaseous phases, beam lines for infrared and far infrared regions, grazing incidence monochromators, temporal structure of SR and its application, and gaseous phase experiments, were held in 1994, 1995, 1996, 1997, 1998, and 2000, respectively. About one third of beam lines have been upgraded in recent years. A Seya-Namioka monochromator at beam line 7B has been replaced by a normal-incidence monochromator to improve a resolving power and spectral range for solid-state spectroscopy. Another Seya-Namioka monochromator at beam line 2B2 has been also replaced by a Dragon-type monochromator for gaseous experiments in VUV and EUV ranges. A multi-layer monochromator installed to the beam line 4A has provided good spectral distribution for photochemical reaction experiments. A 15-m SGM monochromator, which took back of a glancing-incidence monochromator at BL8B1 has been used for solid and gaseous phase experiments with high resolving power in EUV range. A Bruker FT-IR interferometer has been installed to beam line 6A1 besides the old FT-FIR of a Martin-Puplett type, and then the improved system can cover the wide wavelength range from 1 μm to 3 mm. A new monochromator (SGM-TRAIN) constructed at beam line 5A has been used for the experiments on solid and surface with high resolving power. The beam line 2A, which has provided VUV photons for gaseous experiment for a long time, is renewed for the use of the bio-specimens. The beam line 6B, which has been constructed for IR experiments, is under renewal for nano-scale photochemical reaction experiments. The rearrangement of the beam lines 4A and 4B has started to construct high-resolution beam line for gaseous phase at BL4B. The UVSOR has now two soft-x-ray stations equipped with a double-crystal monochromator, eight extreme ultraviolet stations with a glancing incidence or a plane-grating monochromator, four vacuum-ultraviolet stations with a Seya-Namioka-type or a normal incidence-type monochromator, a (far) infrared stations equipped with FT interferometers, a multi-layer monochromator, and four white-light stations without monochromator.

The photoelectron spectroscopy combined with SR is one of the powerful techniques to investigate electronic structures. Several kinds of photoelectron spectrometers are working or ready to work in UVSOR: High-performance electron analyzer at soft x-ray beam line 1A, Two-dimensional spectrometer at VUV beam line 3B, Angle-resolved spectrometer at EUV beam line 8B2, and Spin- and angle-resolved photoelectron spectrometer at helical undulator beam line 5A besides a high-resolution type. Photoelectron microscopy system is under construction at BL6A2, where the optical system is modified to have a good demagnified spot.

In Spring 2000, we had one-month shutdown to replace the first manual valve at BL4A, 4B, 5B, and 6B. The purpose is to install new pre-chamber systems for photochemical reaction and gaseous experiments at BL4A, 4B, and 6B. On this occasion, the vacuum system for FEL experiment was also improved, with the break of the vacuum in the third long straight section.

The examination of the radiation protection system in IMS has been conducted in autumn 1999 by the Ministry of Science and Technology. Since the accident happened at a nuclear-fuel company in 1999, the examination was very strict even for our facility. According to their advice, we had confirmed our radiation protection system. The radiation monitor system was also improved in Spring 2000. The gaseous, dust, and area monitors were renewed since the initial installation in 1983.

There were lots of troubles, as usual, but they did not affect the beam times fortunately. Our interlock valve system could succeed in protecting the storage-ring from the air-leakage at BL3B, and from the accidental electric leakage at BL5B. The alarm/emergency call system and also the education/safety system for beginner users work well. New version of the UVSOR guidebook was published for this purpose. The UVSOR facility strongly asks all users to conduct their experimental procedures according to the beam line manuals and the guidebook.

The persons who want to use the open- and the in-house beam lines are recommended to contact with the stationmaster or supervisor and the representative, respectively. The persons who want to know updated information of the UVSOR facility are requested to open 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 has been replaced from NEC SX-3/34R to combined vector and scalar parallel system of Fujitsu VPP5000 and SGI 2800. VPP5000 system consists of 30 vector CPU-nodes, and has 256 GB of main memory. SGI 2800 has 256 CPU and 256 GB of memory. With the general purpose computer system NEC SX-5 and IBM SP2 installed last year, 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 28% of the computer time is used by the research staff at IMS, and the remaining 72% is given out as research grants to scientists outside the institute in molecular science and related field. As of March 1999, the number of project group was 169, consisting of 659 users.

The library programs of the Center amount to 805. Among them, more than 200 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.