

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 - 1997).

Computer Center

The main computers at the Center are a supercomputer NEC SX-3/34R, NEC HSP(High Speed Scalar Processor), NEC HPC and IBM SP2. The computers are linked to international networks through Science Information Network(SINET). About 30% of the computer time is used by the research staff at IMS, and the remaining 70% is given out as research grants to scientists outside the institute in molecular science and related field. As of March 1998, the number of project group was 188, consisting of 719 users.

In September, 1997, the Hitachi SR2201 parallel CPU Server was installed.

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 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.

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 newly equipped with profitable 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 down 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 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 an important role in the synthesis and purification of chemical substances. The scientists of this facility carry out their own researches on synthesis of new interesting compounds. Upon request, technicians carry out elemental and mass spectrometric analyses. Laboratory waste matters are also managed here. This center continues the task of Low-Temperature Center which supplies liquid helium and liquid nitrogen to the users in IMS. The total amount of liquid helium and nitrogen supplied from June, 1997 to May, 1998 were 42,682 and 64,647 L, respectively. The center is also equipped with various types of instruments such as NMR, ESR spectrometers and X-ray diffractometers for general use.

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 1997 are listed below.

- Chamber for Diagnosing excited oxygen atomic beam
- Sample transferring mechanism for STM
- ^3He refrigerator
- Off-axis parabolic mirror
- Automated measuring program for pressure-dependent electronic resistivity
- Noise canceler for semiconductor laser
- Two-channel two-nanosecond gate pulse generator
- Pulsed magnetic field supply circuit
- 256-channel mid-infrared photodetector

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 four weeks in a year to provide pulsed 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.

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 be added 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 gas phases, beam lines for infrared and far infrared regions, and grazing incidence monochromators were held in 1994, 1995, 1996, and 1997, respectively. About one third of beam lines have been upgraded in a couple of years. A Seya-Namioka monochromator at beam line 7B is being 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 is also under replacement by a Dragon-type monochromator for gaseous experiments in VUV and EUV ranges. A multi-layer monochromator is installed to beam line 4A for photo-chemical reaction experiments. A glancing-incidence monochromator at BL8B1 has been replaced by a 15 m SGM monochromator. This new monochromator having a resolving power of 4,000 at 400 eV is used for solid and gaseous experiments in EUV region. 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 mm to 3 mm. A new monochromator (SGM-TRAIN) has been constructed at beam line 5A for the use of circularly polarized lights from the helical undulator, and is expected to provide a resolving power of 10,000 at 100 eV. 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, two (far) infrared stations equipped with FT interferometers, a multi-layer monochromator, and three 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 lines 6A2 and 8B2, Photoelectron microscopy system at a wiggler beam line 7A (sometimes this system can be used at another beam line 5B), and Spin- and angle-resolved photoelectron spectrometer at helical undulator beam line 5A besides a high-resolution type. The details are given in the UVSOR ACTIVITY REPORT, which is annually published.

There were lots of troubles, especially water-related troubles, in 1997. Since the concrete wall in the basement had many old cracks, the water leakage in the room for electricity happened often in rainy and typhoon seasons. A water pump in the second cooling-circulation system was broken. The pressure in the pre-mirror chamber at BL8B1 became worse suddenly due to a water leakage from the cooling pipe for the pre-mirror. These are common problems to old facilities in the world. On the other hand, we had several troubles due to careless actions by users in 1997. Water from the loosely connected hoses was splashed at BL2A and BL8B2. The air was introduced in the monochromator chamber at BL7A during exchanging specimens. Similar air-leak trouble happened at BL6A1. The viton o-ring in the gate valve was melt during baking procedures at BL8A. These accidents pushed us to confirm the alarm/emergency call system and also the education/safety system for beginner users. The second 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 station master or supervisor and the representative, respectively. The persons who want to know updated informations of the UVSOR facility are recommended to open <http://www.uvsor.ims.ac.jp/>.