Unraveling the mysteries of molecules and extending their possibilities

The aim of the Institute for Molecular Science is to investigate fundamental properties of molecules and molecular assemblies through both experimental and theoretical methods. Since its inception, based on a policy directed to fostering numerous joint programs involving IMS scientists, IMS has made its facilities available to the international scientific community.

Our studies are directed to the design and development of novel materials with new applications and to the advance in innovative methodologies. Molecular reactivities, dynamics, and diverse interactions between different molecules and substances are elucidated.

Our new organization NINS has entered into the fourth year of the incorporation. From the viewpoint of “development of science and culture” which is fundamental for the future national policy in coming hundred years, it would be necessary to reconsider the strategy of research. We, scientists, should strive to improve this situation, and at the same time we have to take this adversity as a spring to carry on basic researches of high quality.

“The construction of network system for efficient use of research equipments in chemistry” requested from IMS has been approved and started as a new program, although the budget for the 2007 fiscal year is very limited. We would like to build up an efficient system for future. The other special programs that IMS undertakes have been successfully carried out. In addition to these, the Asian Core Program in Molecular Science has been approved in the 2006 fiscal year and various activities including collaborative researches and upbringing of young scientists have commenced in cooperation with China, Korea, and Taiwan.

The organization of IMS lasted more than 30 years has been changed from this April. The basic idea is to intensify the cooperative relations between research departments and research facilities, and promote and activate collaborations among various regions. The self-evaluation of the whole institute in the first term of the incorporation is planned to be carried out. As a center of excellence in molecular science all IMS members should strive to further their researches of high originality. We would heartily like to ask for the continuous supports from all the related parties.

NAKAMURA, Hiroki
Message from IMS Director-General
Describing invisible and intricate molecules

Theoretical and Computational Molecular Science

It is our ultimate goal to develop theoretical and computational methodologies that include quantum mechanics, statistical mechanics, and molecular simulations in order to understand the structures and functions of molecules in gasses and condensed phases, as well as in bio and nano systems.

Theoretical Studies of Condensed Phase Dynamics

Motions in liquids and biological systems are intrinsically complicated business. Features of dynamics in these systems are flexibility and hierarchy over a wide range time scales. Understanding these features is indispensable to elucidate the chemical reactions in solutions, the functions of proteins, and the entangled molecular motions in condensed phases. The liquid dynamics and chemical reactions in biological systems are investigated by using molecular dynamics simulation and electronic structure calculation. In addition, analyses based on multi-dimensional spectroscopy are performed to advance our understanding of complicated condensed phase dynamics.

Quantum Dynamics of Proton Transfer in Solution

A quantum mechanical equation of motion for the proton combined with the classical motion of the solvent has been presented in the framework of a mixed quantum-classical molecular dynamics in order to include the quantum effects of the proton. According to this method, we can describe the tunneling and the zero-point energy as well as the vibrational excitation followed by the reaction transition and vibrational relaxation.

Theoretical Studies of Electron Dynamics

Electron dynamics in nanometer-sized molecules and nanostructured materials is an intrinsic process related to a number of interesting phenomena such as linear and nonlinear optical response, electric conduction, and magnetism. Despite its importance, the electron dynamics has not yet been understood. We have developed a computational method simulating the electron dynamics in real time and real space, and revealed the dynamics in detail.

Advanced Electronic Structure Theory for Predictive Quantum Chemistry

Modern electronic structure theory that is practiced with high-performance computers is now capable of supplying analytic interpretation of chemical phenomena, and is being advanced so as to provide predictive information of experiments a priori. The research is aimed at development of a new generation of ab initio quantum chemistry methodology that allows one to describe a wide range of complicated electronic structures, which can be found in conjugated systems or metal complexes, in a predictive chemical accuracy by exploiting cutting-edge theory and sophisticated computing techniques. The resultant method is eventually applied to realistic problems in molecular science.

Imaging and Controlling Molecules Using Intense Laser Pulses

Intense laser fields (~10^19 W/cm^2), comparable with the Coulomb field within atoms and molecules in magnitude, can be generated by focusing high-energy and ultrashort laser pulses. When exposed to such an intense laser field, molecules exhibit various exotic features that are not observed in weak laser fields. Understanding of the behavior of molecules in intense laser fields provides new schemes for the imaging and controlling of ultrafast reaction dynamics.

Light Source Development Using Relativistic Electron Beam

Synchrotron radiation emitted by relativistic electrons in magnetic field is widely used in various research fields, in wide spectral range, from millimeter wave to X-rays. We are developing technologies to produce coherent synchrotron radiation which has optical properties like lasers. We have succeeded in producing coherent radiations in terahertz, visible and ultraviolet region. We are going to explore shorter wavelength region.

Investigation of the Functionality of Materials Using Synchrotron Radiation

Synchrotron radiation is a very bright light source with a bandwidth that extends from the terahertz to X-ray frequencies. Investigations of material functionality under extreme conditions that were previously considered impossible to produce can now be realized using this light source. Of particular interest is the clarification of metal-insulator transitions under high pressure, high magnetic fields and low temperatures as this provides important information for the design of functional materials based on electron correlations.

Create, observe and control with light

Photo-Molecular Science

Molecules respond to photon irradiation in a variety of ways, including photo-induced transitions and photochemical reactions. We have employed various light sources to elucidate molecular structures and properties and to control chemical reactions and molecular functions. We have also developed new and advanced light sources for molecular science.

Real-Time Observations of Ultrafast Nuclear Motions at Solid Surfaces by Nonlinear Spectroscopy

Solid surfaces serve as playgrounds for chemical processes such as corrosion and catalytic reactions. In order to understand reaction mechanisms fully, it is essential to know how adsortbate vibrations and surface phonons are involved in reactions. When adsorbates on a surface are exposed to impulsive stimuli consisting of ultrashort optical pulses, they start vibrating in phase. We have developed a method to monitor these coherent nuclear motions in real time. In addition, we have succeeded in selectively exciting a vibrational motion using tailored pulse trains.
Novel Technique for the Direct Observation of Nano-Magnetic Structures
Magnetic circular dichroism (MCD) photoelectron emission microscopy (PEEM) is a method for the direct observation of nano-magnetic structures with several tens nanometer spatial resolution, and has been broadly utilized by using synchrotron radiation x rays. We discovered however astonishing improvement of the ultraviolet MCD sensitivity by a factor of 10^2 when tuning the wavelength of the ultraviolet lights with a sensitivity similar to that of synchrotron radiation x rays. We are further exploiting nano-scale magnetic domains and domain walls using ultraviolet lights with a sensitivity similar to that of synchrotron radiation x rays. We are further exploiting nano-scale magnetic domains and domain walls using ultraviolet lights with a sensitivity similar to that of synchrotron radiation x rays. We are further exploiting nano-scale magnetic domains and domain walls using ultraviolet lights with a sensitivity similar to that of synchrotron radiation x rays. 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Leading the sustainable future of Japan

--- Grand Challenge in Nanoscience ---

Next Generation Integrated Nanoscience Simulation Software Development & Application of Advanced High-Performance Supercomputer Project Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan

A national project named, "Next Generation Integrated Nanoscience Simulation Software" was initiated on April 1, 2006 at Institute for Molecular Science (IMS). The project is a part of the "Development & Application of Advanced High-Performance Supercomputer Project" of MEXT which aims to develop a next generation supercomputer and application software to meet the nation's computational science needs.

The primary mission of our project is to resolve following three fundamental problems in the field of nanoscience, all of which are crucial to support society's future scientific and technological fundamental problems in the field of nanoscience, all of which are crucial to support society's future scientific and technological needs:

1. "Next Generation Energy" (e.g., effective utilization of the solar energy),
2. "Next Generation Nano Biomolecules" (e.g., scientific contributions toward overcoming obstinate diseases),
3. "Next Generation Nano Information Function and Materials" (e.g., molecular devices).

In these fields, new computational methodologies and programs are to be developed to clarify the properties of nanoscale substances such as catalysts (enzymes), bio-materials, molecular devices, and so forth, by making the best use of the next generation supercomputer.

Formation of Interdisciplinary and International Bases Across Fields of Study

Development of New Computational Methods for Large-Scale Systems and Establishment of Bases for Advanced Simulation of Molecular and Material Systems

This project aims to establish a core computational science base for molecular and material systems and the development of methodologies for advanced calculations. The project has been organized by five institutes within the National Institutes of Natural Sciences, i.e. Institute for Molecular Science, National Astronomical Observatory of Japan, National Institute for Fusion Science, National Institute for Basic Biology, and National Institute for Physiological Sciences, other universities and research institute. We are trying to create a new interdisciplinary field by integrating the different views and methodologies traditionally associated with each of the fields that belong to different hierarchies within the natural sciences. Structures and dynamics of large-scale complex systems, such as nanomaterials and biological systems, are investigated by using a variety of sophisticated computational methods based on theories of electronic structure, statistical mechanics, and so on. The development of new computational methods and cooperation on improving the efficiency of calculations utilizing parallel operations have also been furthered as a consequence of the members having different scientific backgrounds.

Extreme Photonics

We have initiated this project in close collaboration with the RIKEN Institute to promote photo-molecular science, which has the potential to contribute significantly to a variety of disciplines including the nano molecular sciences and life sciences. This project includes new studies directed at developing new coherent light sources, new microspectroscopic methods, and controlling molecular dynamics through optical phase manipulation with ultrahigh precision.

--- Special Programs ---

MEXT Nanotechnology Network

Nanotechnology Support Project in Central Japan: Synthesis, Nanoprocessing and Advanced Instrumental Analysis

The Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan started the Nanotechnology Network Project in 2007 in order to support Japan's nanotechnology researches not only from universities and government institutes but also from private companies. IMS participates in this project with Nagoya University, Nagoya Institute of Technology and Toyota Technological Institute, and establishes a nanotechnology support center in central Japan area. We will support:

1) Public usage of various advanced nanotechnology instruments such as ultrahigh magnetic field NMR (900 MHz), advanced transmission electron microscopes, and so forth
2) design, synthesis and characterization of organic, inorganic and biological molecules and materials,
3) semiconductor nanoprocessing using advanced facilities and technologies.

We will promote applications not only to each supporting element, but to combined usage of several elements such as a nanobiochemistry field that is highly efficient in this joint project.

Inter-University Network for Efficient Utilization of Chemical Research Equipments

Academic and industrial activities in Chemistry in Japan have been highly influential over the past 30 years. Needless to say, it is highly important to improve the supporting environment for research and education in science and engineering. In particular, research equipments advances all the time to more intelligent and expensive ones, making measurement time shorter with higher reliability. It would be economic and efficient for the researchers and students of all national universities to share such equipments for performing high level research and education.

On April 7th 2007, the selected representatives from 72 universities gathered in Oizaki and decided to start the Inter-University Network for Efficient Utilization of Chemical Research Equipments. This system is operated through internet machine-time reservation and charging system by the help of equipment managers and accounting sections in each university. All the universities are grouped into 12 regions and in each region the hub university organizes the regional committee for the operation of regional network system. There is no barrier for every user to access to any universities beyond his/her regional group. We believe that this innovative system can motivate and stimulate researchers and students to carry out new researches, and make chemistry research in Japan far more successful and active.

State-of-the-art facilities supporting cutting-edge research

UVSOR Facility

Vacuum ultraviolet (VUV) light is not alive when the solar light reaches the earth, because molecules in the air have strong interaction with VUV. The wavelength of the VUV light is between ultraviolet (UV) light and X-rays. Since VUV light is indispensable in photon science of molecules it is artificially produced. Institute for Molecular Science constructed a circular accelerator based on the synchrotron radiation (SR) mechanism in 1983. In 2003, we upgraded the accelerator to achieve the world’s highest brilliance of small SR facilities. The next generation soft X-ray emission spectrometer was recently successfully developed. Our SR facility is called UVSOR.
Research Center for Molecular Scale Nanoscience
The Center was established in 2002 with the mission of undertaking comprehensive studies of "Molecular Scale Nanoscience." The Center consists of one division staffed by full-time researchers, two divisions staffed by adjunctive researchers, one division staffed by visiting researchers. Their mandates are: (1) fabrication of new nanostructures based on molecules; (2) systematic studies of unique chemical reactions and physical properties of these nanostructures. The Center administers offer public usage of the advanced ultra-high magnetic field NMR (Nuclear Magnetic Resonance, 900 MHz) spectrometer. Moreover, the center conducts the Nanotechnology Network Project of the Ministry of Education, Culture, Sports, Science and Technology (MEXT) as a core organization, and provides various kinds of nanotechnology programs.

Laser Research Center for Molecular Science
The center aims to develop new experimental apparatus and methods to open groundbreaking research fields in molecular science, in collaboration with the Department of Photo-Molecular Science. Those new apparatus and methods will be served as key resources in collaboration with the Department of Photo-Molecular Science. Those new apparatus and methods will be served as key resources in advanced collaborations with the researchers from the community of molecular science. The main targets are: (1) advanced photon sources covering wide energy ranges from terahertz to soft X-ray regions; (2) molecular science. The main targets are (1) advanced photon sources covering wide energy ranges from terahertz to soft X-ray regions; (2) molecular science.

Instrument Center
This center is established in 2007 combining the general-purpose instruments of the Research center for molecular-scale nanoscience and Laser research center for molecular science. The main instruments are: NMR, mass spectrometer, powder X-ray diffractometer, dilution refrigerator with superconducting magnet, fluorescence spectrophotometer, UV-VIS-NIR spectrophotometer, circular dichroic spectrometer in Myodaiji campus. We mainly support a general-use experiment, and we often support a special one such as the experiment combining lasers and general-purpose machines. We provide liquid nitrogen and liquid helium using helium liquefiers. We also support the network sharing system of the chemistry-oriented instruments, which starts in the April of 2007.

Equipment Development Center
We are developing various kinds of apparatus and devices required for conducting molecular science experiments, either by ourselves or through collaborations with in-house and outside scientists. Facilities for mechanical, electronics and glass works are well established, and the requirements of advanced research initiatives in molecular science are supported by these facilities based on the high level of technology that has been developed since the establishment of IMS. It is our mission to provide the technological environment necessary for supporting highly innovative research through facilitating the consultative process between the scientist and the engineer.

Okazaki Institutes for Integrative Bioscience
The main purpose of the Okazaki Institutes for Integrative Bioscience (OIB) is to conduct interdisciplinary research in the molecular sciences, basic biological sciences, and physiological sciences. The OIB employs cutting edge methodologies from the physical and chemical disciplines to foster new trends in bioscience research. The OIB is a center shared by and that benefits from all three of the institutes in Okazaki. Three full professors and one associate professor, all of whom are members of IMS, staff the OIB.

Research Center for Computational Science
High-quality hardware and software services are provided to the scientists in our country in the field of molecular science and bioscience. Pioneering large-scale quantum chemical and molecular dynamics calculations are conducted using our super computer systems "Grid Computing System" and "Super-High-Performance Molecular Simulator." Totally, they have performance as high as near 20 TFLOPS. A new supercomputer system will be introduced further this fiscal year to realize much higher computational environment.

Instrument Center
This center is established in 2007 combining the general-purpose instruments of the Research center for molecular-scale nanoscience and Laser research center for molecular science. The main instruments are: NMR, mass spectrometer, powder X-ray diffractometer, dilution refrigerator with superconducting magnet, fluorescence spectrophotometer, UV-VIS-NIR spectrophotometer, circular dichroic spectrometer in Myodaiji campus. We mainly support a general-use experiment, and we often support a special one such as the experiment combining lasers and general-purpose machines. We provide liquid nitrogen and liquid helium using helium liquefiers. We also support the network sharing system of the chemistry-oriented instruments, which starts in the April of 2007.

Serving as a core organization for domestic research
Joint Study Programs
As one of the important functions of an inter-university research institute, IMS facilitates joint study programs for which funds are available to cover the costs of research expenses as well as the travel and accommodation expenses of individuals. Proposals from domestic scientists are reviewed and selected by an inter-university committee.

The programs are conducted under one of the following categories:
(1) Joint Studies on Special Projects (a special project of significant relevance to the advancement of molecular science can be carried out by a team of several groups of scientists).
(2) Research Symposia (a symposium on timely topics organized as a collaborative effort between outside and IMS scientists).
(3) Cooperative Research (a research program conducted by outside scientists with collaboration from an IMS scientist).
(4) Use of Facilities (a research program conducted by outside scientists using the research facilities of IMS).
(5) Invited Research Project.
(6) Joint Studies Programs using beam lines of the UVSOR Facility.
(7) Use of Facilities in the Research Center for Computational Science (research programs conducted by outside scientists at research facilities in the Research Center for Computational Science).
International communication and cooperation

**International Collaboration and International Exchange**

IMS has accepted many foreign scientists and hosted numerous international conferences since its establishment and is now universally recognized as an institute that is open to foreign counties. In 2004, IMS initiated a new program to further promote international collaboration. As a part of this new program, IMS faculty members can, (1) nominate senior foreign scientists for short-term visits, (2) invite young scientists for long-term stays and, (3) undertake visits overseas to conduct international collaborations. In 2006, IMS started a new program, JSPS Asian CORE Program on “Frontiers of material, photo- and theoretical molecular sciences” (2006-2010). This new program aims to develop a new frontier in the molecular sciences and to foster the next generation of leaders through the collaboration and exchange among IMS and core Asian institutions: ICCAS (China), KAIST (Korea) and IAMJS (Taiwan).

Highly capable personnel nurtured by abundant research resources

**Personnel Training : Education in Graduate School**

**What is SOKENDAI?**

The Graduate University for Advanced Studies (hereafter referred to as “SOKENDAI”) was founded in 1988 with the intention of cultivating new integrative research fields and to promote academic excellence through its doctoral course programs. They are also open to foreign students. The university is based in the town of Hayama in Kanagawa Prefecture, Japan, and its unique education programs are currently available in Hayama, as well as at eighteen other national academic research institutes to which individual students are assigned according to their field of study.

**Personnel and Budget**

**Administrative Council**

**Director:**

- **ESAKI, Nobuyoshi**
- **KATO, Shinnichi**
- **TSUCHIYA, Soji**
- **NODUCHI, Hiroshi**
- **MILLER, H. William**
- **LAUBEREU, Alfred**

**Research Consultants**

- **HIROTA, Noboru**
- **KONDO, Tamotsu**
- **TAMAO, Kohei**

**Advisory Committee**

- **AWAGA, Kunio**
- **ENOKI, Toshiaki**
- **FUJITA, Makoto**
- **KATO, Masakazu**
- **MAEKAWA, Sadamichi**
- **NAKAMURA, Atsushi**
- **SEKIYA, Hiroshi**
- **TANAKA, Kenichirou**
- **TERAZIMA, Masahide**
- **YAMASHITA, Kouichi**
- **HIRATA, Fumio**
- **KOSUGI, Nobuhiro**
- **NAGASE, Shigeru**
- **NISHI, Nobuyuki**
- **OGAWA, Takaji**
- **OKAMOTO, Hiroshi**
- **OHMORI, Kenji**
- **TANAKA, Koji**
- **URISU, Tsuneo**
- **YAKUSHI, Kyuya**
- **YOKOYAMA, Toshihiko**

**Okazaki Library and Information Center**

[http://www.lib.or.jp/]

In the Okazaki Library and Information Center, books and journals from three affiliated institutes (IMS, NIBB, NIFS) are collected, arranged and stored for the convenience of staff and visiting users.

**Okazaki Conference Center**

[http://www.orion.or.jp/loc/cen2/]

The Okazaki Conference Center was founded in February 1997 for the purposes of hosting international and domestic academic exchanges, developments in research and education in the three Okazaki Institutes, as well as the promotion of social cooperation. An auditorium (Daikaigisha-shitsu), a middle room (Chu-kaigisha-shitsu) and two small rooms (Sho-kaigisha-shitsu) with seating capacities of 250, 100, and 50, respectively, are available.

**Visiting Foreign Researchers (2006)**

![Visiting Foreign Researchers](image)

**Common Facilities in Okazaki**

- Dormitories for Visiting Researchers
  - For visiting researchers from universities and institutes within Japan and all over the world, the dormitory called the Mishima Lodge is available. It takes 10 minutes on foot from the Myodaiji area to the Mishima Lodge.

**Okazaki Library and Information Center**

[http://www.lib.or.jp/]

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<tr>
<th>Available services</th>
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<tr>
<td>Library is open 24 hours using ID cards.</td>
</tr>
<tr>
<td>Online reading of journals and searching using Web of Science, SciFinder Scholar, etc.</td>
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**Budget (2006)**

<table>
<thead>
<tr>
<th>Grant-in-Aid (2006)*</th>
<th>(Thousand yen)</th>
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<tbody>
<tr>
<td>Total</td>
<td>3,154,912</td>
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<tr>
<td>CREST, PRESTO, others**</td>
<td>32,500</td>
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<tr>
<td>Special Coordination Funds for Promoting Science and Technology from MEXT**</td>
<td>509,907</td>
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<td>Others**</td>
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<td>Total</td>
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<tr>
<th>Grants-in-Aid (2006)*</th>
<th>(Thousand yen)</th>
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<tr>
<td>Total</td>
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<td>CREST, PRESTO, others**</td>
<td>395,564</td>
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<tr>
<td>Special Coordination Funds for Promoting Science and Technology from MEXT**</td>
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