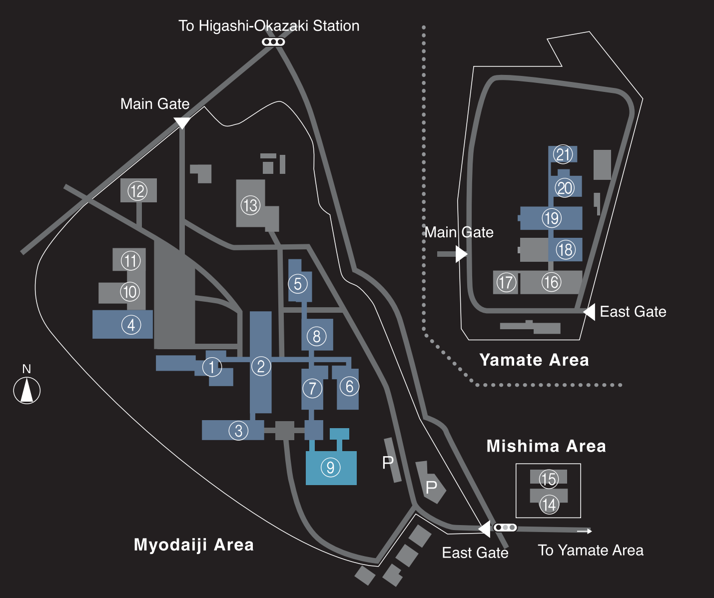
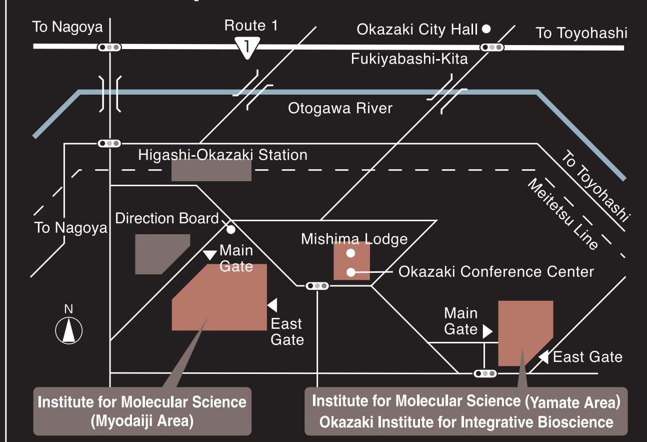
NATIONAL INSTITUTES OF NATURAL SCIENCES
Institute for Molecular Science
Myodaiji Area: 38 Nishigo-Naka, Myodaiji, Okazaki 444-8585, Japan
Yamate Area: 5-1 Higashiyama, Myodaiji, Okazaki 444-8787, Japan
Phone: +81-564-55-7000 FAX: +81-564-54-2254
http://www.ims.ac.jp/

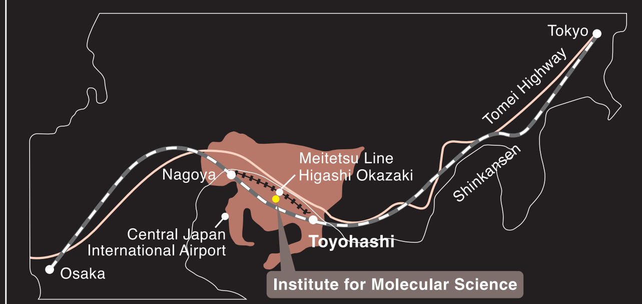
Campus Map



	(m²)
① Research Facilities	2,752
② Laboratories	8,857
③ Southern Laboratories	3,935
④ Research Center for Computational Science	2,474
⑤ Low-Temperature Center	1,527
⑥ Chemical Material Center	1,063
⑦ Laser Center	1,053
⑧ Equipment Development Center	1,260
⑨ UVSOR Facility	3,097
⑩ Administration office	2,371
⑪ Library	2,002
⑫ Staff Hall	1,575
⑬ Energy Center	1,255
⑭ Okazaki Conference Center	2,863
⑮ Mishima Lodge	4,079
⑯ Yamate No.1 Bldg. A	4,674
⑰ Yamate No.1 Bldg. B	2,303
⑱ Yamate No.2 Bldg.	8,453
⑲ Yamate No.3 Bldg.	10,757
⑳ Yamate No.4 Bldg.	3,813
㉑ Yamate No.5 Bldg.	664

Access Map





From Tokyo

At Toyohashi Station, catch the Meitetsu train and get off at Higashi-Okazaki Station (approx. 20 min from Toyohashi to Higashi-Okazaki). Turn left at the ticket gate and walk south for approx. 7 min.

From Osaka

At Meitetsu Nagoya Station, catch the Meitetsu train and get off at Higashi-Okazaki Station (approx. 30 min from Meitetsu Nagoya to Higashi-Okazaki).Turn left at the ticket gate and walk south for approx. 7 min.

From Central Japan International Airport (Centrair)

By Train
Catch the Meitetsu train at Central Japan International Airport Station and get off at Higashi-Okazaki Station (approx. 65 min from the Central Japan International Airport Station to Higashi-Okazaki). Turn left at the ticket gate and walk south for approx. 7 min.
By Bus
Catch the Meitetsu bus at Central Japan International Airport and get off at Higashi-Okazaki Bus Station (approx. 65 min from the Airport to Higashi-Okazaki). You are on the north side of the Meitetsu Higashi-Okazaki Station. Go through the passage connecting the south side of the Higashi-Okazaki Station and further walk south for approx. 7 min.

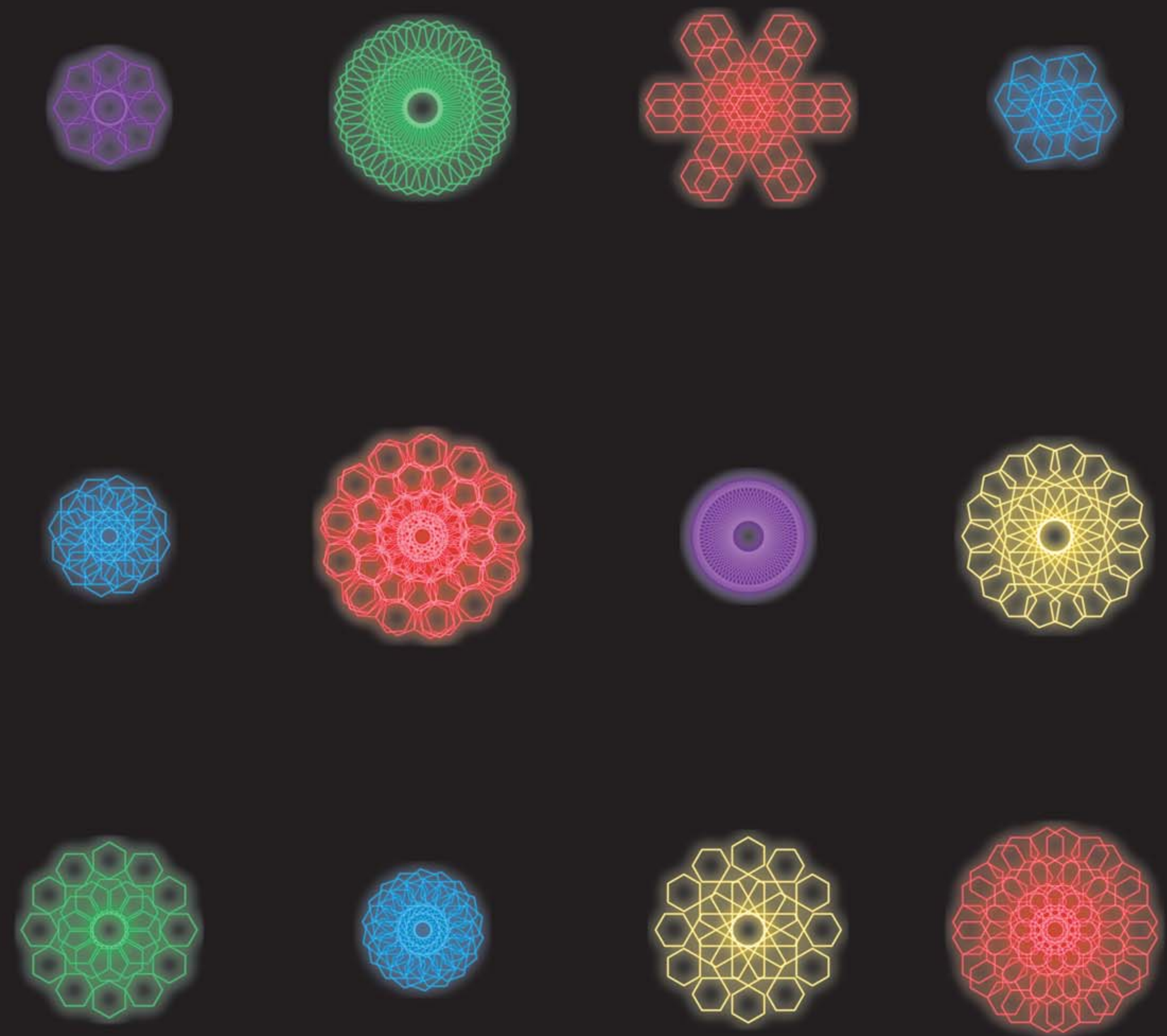
By Car

Take the Okazaki Exit on the Tomei Highway. Approx. 1.5 km toward Nagoya, turn left at the Fukiyabashi-Kita turnoff (approx. 10 min from Okazaki Exit).

2007.7

NATIONAL INSTITUTES OF NATURAL SCIENCES

IMS [Institute for Molecular Science]



2007

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 view-point 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 structure by analyzing the problems we have faced. The present situation of Japanese science policy is unfortunately quite serious. 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.

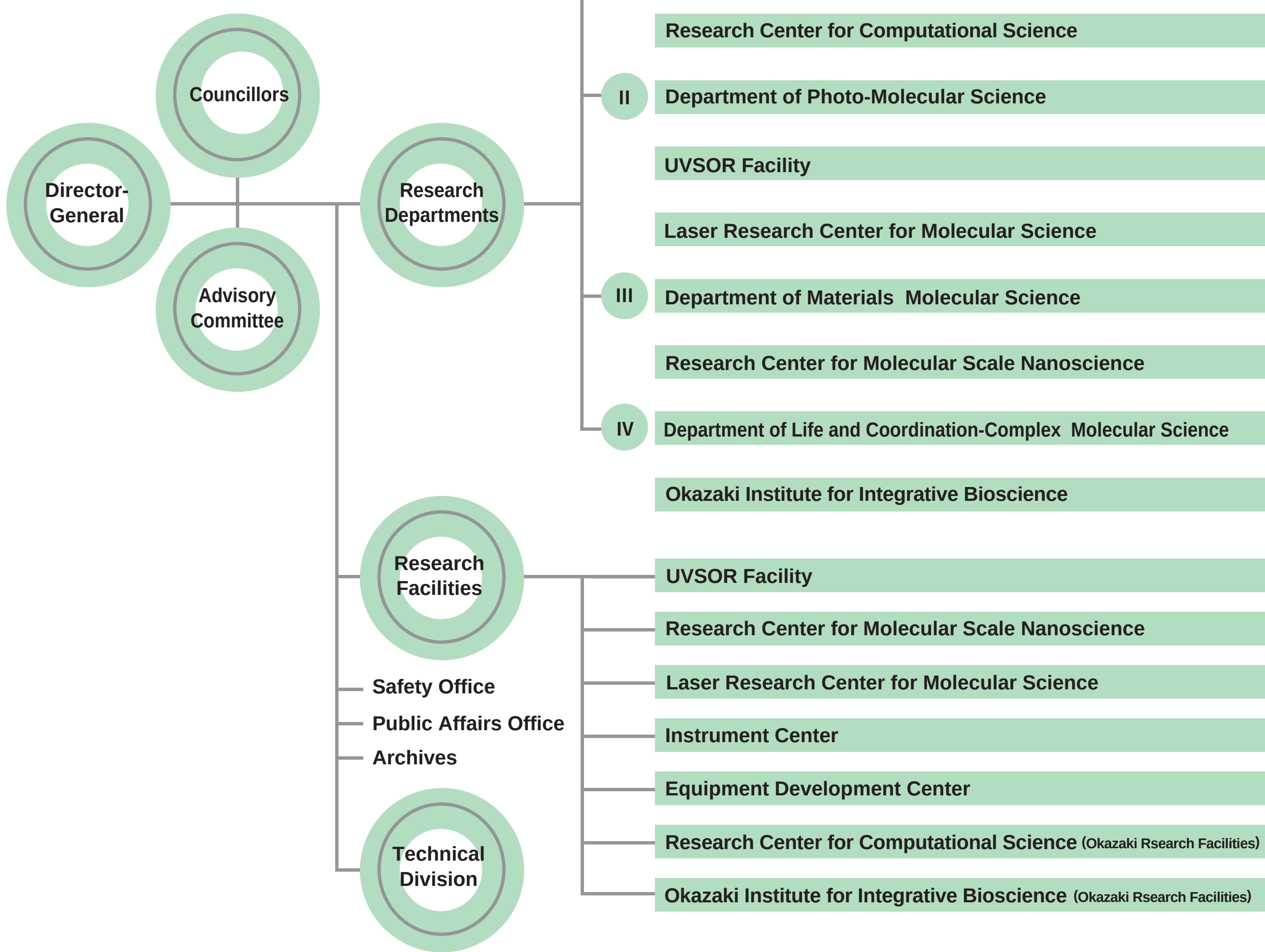
The organization of IMS lasted more than 30 years has been changed from this April. The basic idea is to intensify the cooperative relations between research departments and research facilities, and promote and activate collaborations among various regions. The self-evaluation of the whole institute 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

[ORGANIZATION]

Institute for Molecular Science



Organization

Research groups at the Institute for Molecular Science belong to Departments or Research Facilities. Technical groups primarily belong to one of the research facilities and have been responsible for energy conservation, safety, security, the information network, public affairs, and other such functions, since the agencization, or privatization, of IMS started in April 2004. Together with the National Institute for Basic Biology and the National Institute for Physiological Sciences, IMS manages the Okazaki Research Facilities on the same Okazaki campus. All of these institutes belong to the National Institutes of the Natural Sciences, which is one of the Inter-University Research Institutes. All of the IMS research groups, including three research groups at the Research Center for Computational Science and four research groups of the Okazaki Institute for Integrative Bioscience in the Okazaki Research Facilities, support visiting researchers from national, public and private universities in Japan. The nature of these joint research initiatives are beyond the framework of their respective universities and allows these researchers use the state-of-the-art facilities and equipment available in the field of molecular science.

History

Apr. 1975	Institute for Molecular Science founded (April 22, 1975) Instrument Center established (-March 1997) Equipment Development Center established
May. 1976	Chemical Materials Center established (-March 1997)
Apr. 1977	Computer Center established (-March 2000) Low-Temperature Center established (-March 1997)
Apr. 1981	Okazaki National Research Institutes (ONRI) founded
Apr. 1982	UVSOR Facility established
Apr. 1984	Coordination Chemistry Laboratories established (-March 2007)
Oct. 1988	Graduate University of Advanced Studies founded School of Mathematical and Physical Science, Department of Structural Molecular Science/ Department of Functional Molecular Science established
Apr. 1997	Laser Research Center for Molecular Science established Research Center for Molecular Materials established (-March 2002)
Apr. 2000	Research Facilities (Okazaki Institute for Integrative Bioscience and Research Center for Computational Science) established
Apr. 2002	Research Center for Molecular-scale Nanoscience established
Apr. 2004	National Institutes of Natural Sciences founded as one of the four Inter-University Research Institute Corporations
Apr. 2007	7 Departments recognized to 4 Departments Instrument Center re-established

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.

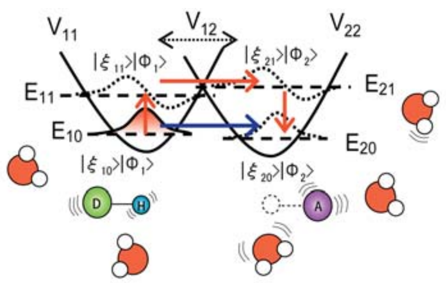
Theoretical Studies of Condensed Phase Dynamics

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.

Signal transduction protein, Ras.

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.

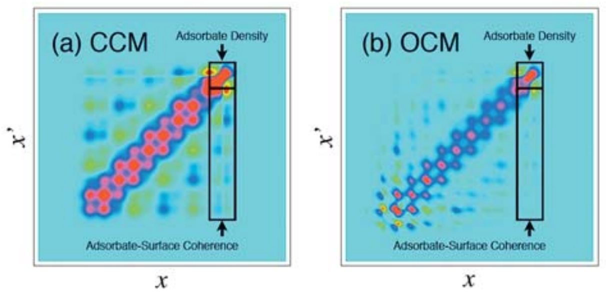


$$i\hbar\dot{C}_{ml}(t) = E_{ml}C_{ml}(t) + \sum_{n(\neq m)}\sum_{k}\langle\xi_{ml}|V_{mn}|\xi_{nk}\rangle C_{nk}(t) - i\hbar\sum_{k}\langle\xi_{ml}|\dot{\xi}_{mk}\rangle C_{mk}(t)$$

Quantum mechanical equation of motion for the proton in solution.

Theoretical Studies of Electron Dynamics

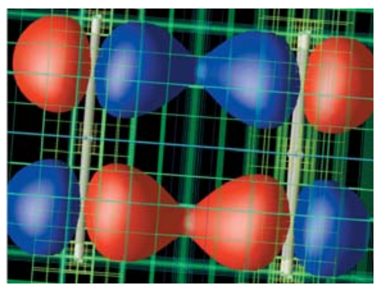
Electron dynamics in nanometer-sized molecules and nanostructured materials is an intrinsic process related to a number of interesting phenomena such as linear and nonlinear optical response, electric conduction, and magnetism. Despite its importance, the electron dynamics has not yet been understood.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



One-body reduced density matrix of an adsorbate-surface system in real space representation.

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.



Multiresolution representation of a molecular orbital of benzene dimer.

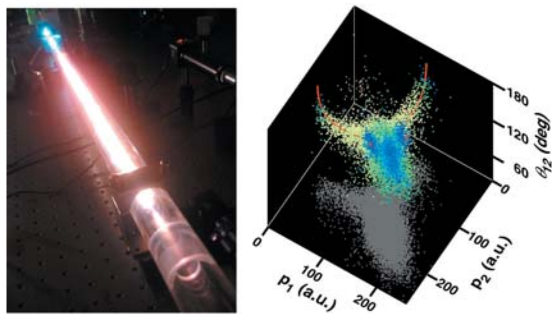
Create, observe and control with light

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 slso developed new and advanced light sources for molecular science.

Imaging and Controlling Molecules Using Intense Laser Pulses

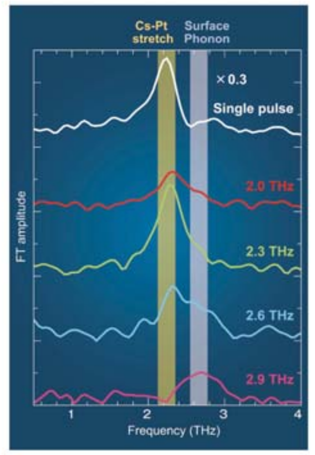
Intense laser fields (~10^{15} W/cm^2), comparable with the Coulomb field within atoms and molecules in magnitude, can be generated by focussing high-energy and ultrashort laser pulses. When exposed to such an intense laser field, molecules exhibit various exotic features that are not observed in weak laser fields. Understanding of the behavior of molecules in intense laser fields provides new schemes for the imaging and controlling of ultrafast reaction dynamics.

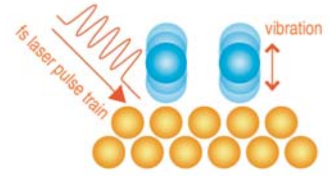


(Left) Generation of sub-10 fs ultrashort intense laser pulses.
(Right) Three-dimensional momentum correlation map for CS_2 in intense laser fields.

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 adsorbate 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.

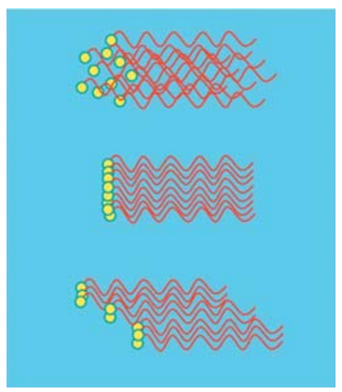




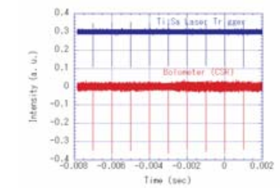
Control of nuclear vibration at a surface using tailored optical pulses.

Light Source Development Using Relativistic Electron Beam

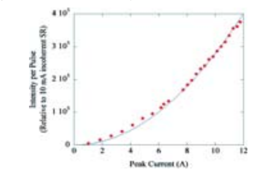
Synchrotron radiation emitted by relativistic electrons in magnetic field is widely used in various research fields, in wide spectral range, from millimeter wave to X-rays. We are developing technologies to produce coherent synchrotron radiation which has optical properties like lasers. We have succeeded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



Normal synchrotron radiation (upper) and coherent synchrotron radiation (lower).



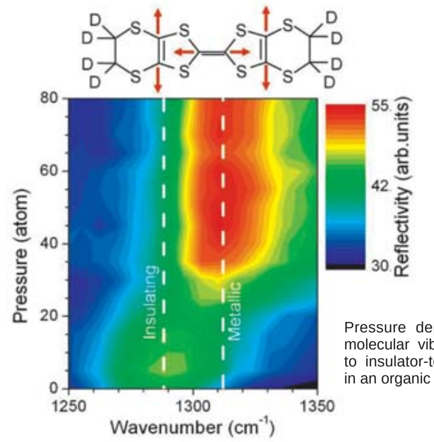
By creating a micro-structure on an electron pulse using an external laser, we can produce coherent synchrotron radiation.



The intensity of the coherent synchrotron radiation is proportional to the square of the electron beam intensity.

Investigation of the Functionality of Materials Using Synchrotron Radiation

Synchrotron radiation is a very brilliant 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.



Pressure dependence of the molecular vibration mode due to insulator-to-metal transition in an organic material.

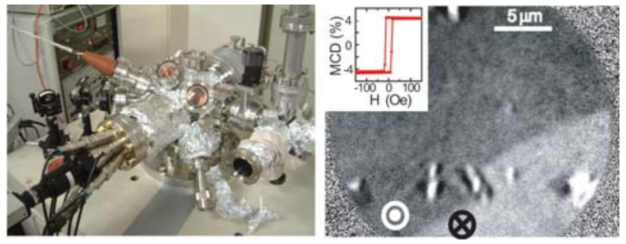
Materials development, functional control and developping new measurement techniques

Materials Molecular Science

Extensive development of new molecules, molecular systems and their higher-order assemblies is being conducted. Their electric, photonic and magnetic properties, reactivities, and catalytic activities are being examined in an attempt to discover new phenomena and useful functionalities.

Novel Technique for the Direct Observation of Nano-Magnetic Structures

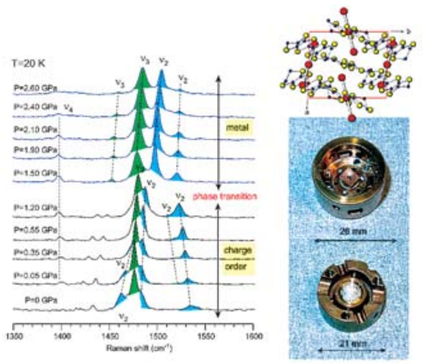
Magnetic circular dichroism (MCD) photoelectron emission microscopy (PEEM) is a method for the direct observation of nano-magnetic structures with several tens nanometer spacial resolution, and has been widely utilized by using synchrotron radiation x rays. We discovered however astonishing improvement of the ultraviolet MCD sensitivity by a factor of 10^2 when tuning the wavelength of the ultraviolet lights. This allows us to perform in-laboratory measurements of the 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 a femto-second time resolved apparatus by virtue of short-pulsed lasers, which is hardly achievable by using synchrotron radiation.



High-sensitive MCD PEEM apparatus using ultraviolet lasers (left), and ultraviolet MCD PEEM image of Cs-coated 12 monolayer Ni films on Cu(001). A HeCd laser (wavelength 325 nm) was used, and the diameter of the image is 25 m. The dark and bright parts correspond to the upward and downward magnetic domains, respectively.

Observation of the Electronic Phase by Raman Spectroscopy

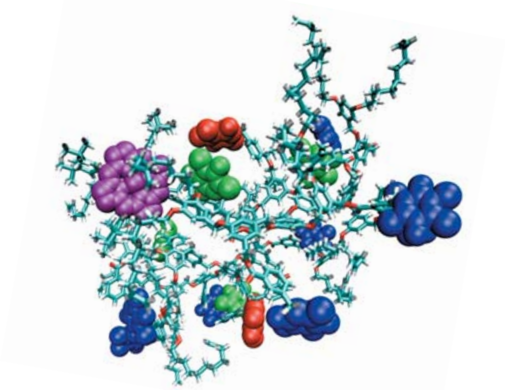
Temperature and pressure often change the electronic properties of materials drastically. If we investigate the properties under various temperature and pressure, we can make a map of the properties (electronic phase diagram). The electronic phase diagram plays an important role in understanding the material's properties and developing new materials. Utilizing the Raman spectroscopy, we are investigating the electronic phase diagram of organic conductors, especially focusing on the electronic phase neighboring on a superconducting phase.



Pressure dependence of the Raman spectrum of an organic conductor at 20 K. 1 GPa corresponds to 10^4 bar. This compound changes into metallic state above 1.5 GPa. Right figure shows a tool to generate high-pressure.

Building Photosynthesis from Artificial Molecules

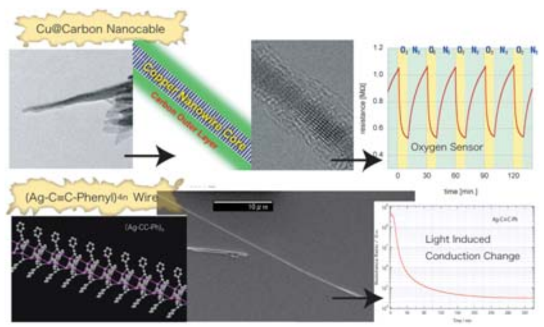
Plant photosynthesis utilizes solar energy by combination of chemical reactions. The machinery is extraordinarily complex, however it is made entirely from molecules. This is a challenge for us molecular scientists to confront. We are currently developing molecular parts for building artificial photosynthetic systems from scratch. Such studies will eventually lead us to the mysterious zone between life and materials.



A single-molecular quinone pool.
It stores the photochemical energy via chemical conversion within the molecule.

Designing of Nano-Structures with Metal-Carbon, Metal-Aromatic Molecule Interfaces

Various novel functions can be produced by utilizing the interfaces between a metal-nanowire or particle core and a carbon or aromatic mantle layer of hybrid nano-composites. This interface is called Schottoky barrier producing large potential gradient. Carbon nanolayers covering the copper nanowire cores exhibit large electric conductivity increment upon oxygen physical adsorption. The increment obeys Langmuir adsorption isotherm and the conductivity change is reproducible. The oxygen molecules donate holes into the system.



Left column: Electric resistance change of a thin tablet of copper nanocables with a carbon outer layer upon repetitive N_2/O_2 exchange. Right column: Dramatic increase in electric conductance for light irradiation on a casted molecular crystals of phenylethynyl silver ultralong molecules.

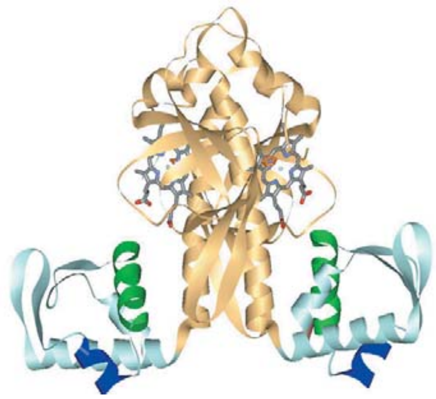
Realizing vital functions and efficient chemical reactions

Life and Coordination-Complex Molecular Science

We are undertaking researches to elucidate the molecular mechanisms responsible for various biological functions and to develop new molecular devices using biological molecules. We are also working on energy-material conversion, organic molecules transformation in water, and activation of small inorganic molecules with high efficiencies by using metal complexes aimed for the reduction of environmental burdens.

The Regulation of Biological Function by Metalloproteins

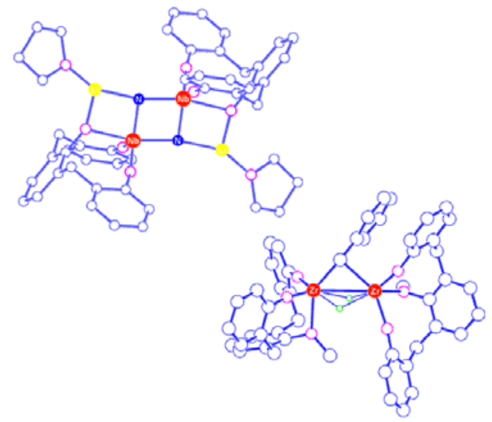
Metalloproteins play an important role for energy metabolism, molecular metabolism, and signal transduction in biological systems. The elucidation of the structure and function of these metalloproteins is central to understanding the regulatory mechanisms associated with biological functioning. We are currently elucidating the structure-function relationships of metalloproteins using experimental methods in the areas of biochemistry, molecular biology, organic chemistry, inorganic chemistry, and physical chemistry.



Structure of the CO-sensor protein containing an iron-porphyrin complex.

Design of Metal Complexes Capable of Activating Small Molecules

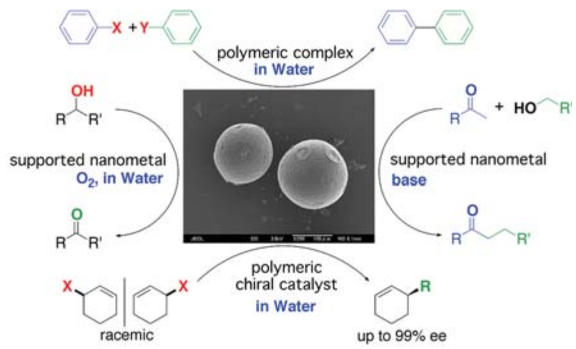
The efficient activation of small molecules such as dinitrogen, carbon monoxide, and carbon dioxide under mild conditions is a challenging topic in chemistry because of their important applications. We are working on the synthesis and structures of new coordination and organometallic compounds of transition metals. One of ongoing works in our lab now concerns the design of novel complexes capable of mediating unusual transformations. For instance, our group has discovered that early transition metal hydride complexes bearing aryloxide ligands can readily cleave dinitrogen and carbon monoxide.



Metal complexes capable of activating small molecules.

Heterogeneous Acuacatalytic System

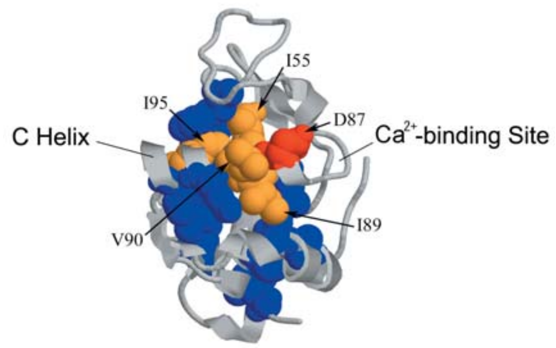
Various types of catalytic organic molecular transformations, e.g. carbon-carbon bond forming cross-coupling, carbon-heteroatom bond forming reaction, aerobic alcohol oxidation, *etc*., were achieved in water under heterogeneous conditions by using amphiphilic polymer-supported transition metal complexes and nanoparticles, where self-concentrating behavior of hydrophobic organic substrates inside the amphiphilic polymer matrix played a key role to realize high reaction performance in water.



A typical SEM image of the amphiphilic polymeric catalysts and the representative aquacatalyses.

To Explore How a Protein Acquires Its Native Three-Dimensional Structure

How does a protein acquire its functional stereo-regular structure based on the amino-acid sequence (= genetic information)? Because of such interest, we are studying (1) the refolding processes of proteins *in vitro*, and (2) the reaction mechanisms of molecular chaperones that are related to protein folding. To this end, we use various spectroscopic techniques including NMR, other physical techniques such as calorimetry, and molecular biological techniques including gene-manipulation experiments.



The folding initiation site of a model protein, α-lactalbumin (orange and red space-filling atoms).

Researchers in the forefront of Molecular Science

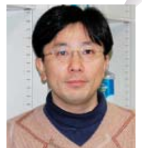
Department of Theoretical and Computational Molecular Science

NAGASE, Shigeru
Theory and Computation of Molecular Design and Reaction

NOBUSADA, Katsuyuki
Theoretical Studies of Dynamics in Quantum Many-Particle Systems

HIRATA, Fumio
Theoretical Studies on Chemical Processes in Solutions Based on the Statistical Mechanics

YANAI, Takeshi
Advanced Quantum Chemistry Modeling and Its Simulation for Molecular Electronic Structures



SAITO, Shinji
Theoretical Study on Dynamics and Spectroscopy in Condensed Phases

YONEMITSU, Kenji
Condensed Matter Theory for Low-Dimensional Molecular Conductors

Research Center for Computational Science

OKAZAKI, Susumu
Molecular Simulation of Complex Classical Systems and Quantum Dynamics of Systems in Condensed Phase

UVSOR Facility

KATOH, Masahiro
Light Source Development Using Relativistic Electron Beam

KIMURA, Shin-ichi
Synchrotron Radiation Spectroscopy on Functional Materials

SHIGEMASA, Eiji
Dynamics of Molecular Inner-Shell Processes

Department of Photo-Molecular Science

OKAMOTO, Hiromi
Spectral and Dynamic Imaging of Photoexcited Nanomaterials

KOSUGI, Nobuhiro
Soft X-ray Photophysics and Photochemistry: Inner-Shell Excitation Dynamics

OHSHIMA, Yasuhiro
Quantum-State Manipulation of Molecular Motions

MITSUKE, Koichiro
Photoionization and Photofragmentation Dynamics in the Extreme Ultraviolet

OHMORI, Kenji
Attosecond Quantum Engineering

HISHIKAWA, Akiyoshi
Imaging and Controlling Molecular Reactions by Ultrashort Intense Light Pulses

Laser Research Center for Molecular Science

TAIRA, Takunori
Micro Solid-State Photonics

Department of Materials Molecular Science

NISHI, Nobuyuki
From Cluster Science to Construction of Functional Metal-Molecule Nano-composites

TSUKUDA, Tatsuya
Studies on Structures and Functions of Metal Nanoclusters

YOKOYAMA, Toshihiko
Preparation and Characterization of Novel Magnetic Thin Films and Exploitation of New Magneto-Optical Techniques

NAKAMURA, Toshikazu
Magnetic Resonance Investigations of Electronic Properties in Molecular-Based Solids

YAKUSHI, Kyuya
Solid State Properties of Molecular Conductors

JIANG, Donglin
Design and Functions of Novel Dendritic Metallo-Arrays

NISHIMURA, Katsuyuki
A New Development of Solid-State NMR Methodology to Reveal 3D Structure and Dynamics for Biomolecules

Research Center for Molecular Scale Nanoscience

OGAWA, Takuji
Creation of Molecular Nano Structures for Molecular Electronics

SUZUKI, Toshiyasu
Organic Semiconductors for Electronic Devices

NAGATA, Toshi
Construction of Complex Chemical Systems Inspired by Photosynthesis

SAKURAI, Hidehiro
Chemistry of Buckybowls and Heterofullerenes

KATO, Koichi
Structural Analyses of Biological Macromolecules by Ultra-High Field NMR Spectroscopy

Department of Life and Coordination-Complex Molecular Science

URISU, Tsuneo
Ionchannel Biosensor

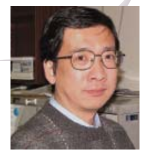
OZAWA, Takeaki
Development of Methods to Analyze Biomolecular Dynamics in Living Cells

UOZUMI, Yasuhiro
Development of Transition Metal-Based Synergistic Catalyst Systems

KAWAGUCHI, Hiroyuki
Design and Synthesis of Metal Complexes to Activate Small Molecules

TANAKA, Koji
Designing and Preparation of Metal Complexes Aimed at Reversible Conversion between Electrical and Chemical Energies

Okazaki Institute for Integrative Bioscience



AONO, Shigetoshi
Structure and Function of Novel Metalloproteins

KUWAJIMA, Kunihiro
Elucidation of the Mechanism of Protein Folding

FUJII, Hiroshi
Molecular Mechanism of Metalloproteins and Metalloenzymes

Leading the sustainable future of Japan

— Grand Challenge in Nanoscience —

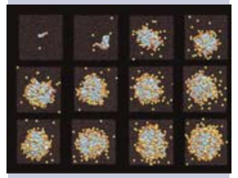
Next Generation Integrated Nanoscience Simulation Software Development & Application of Advanced High-Performance Supercomputer Project Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan

A national project named, "Next Generation Integrated Nano-science 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 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), and (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 devises, and so forth, by making the best use of the next generation supercomputer.

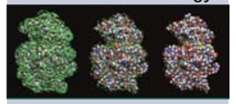
Next Generation Nano Information Function and Materials

Next Generation Nano Biomolecules

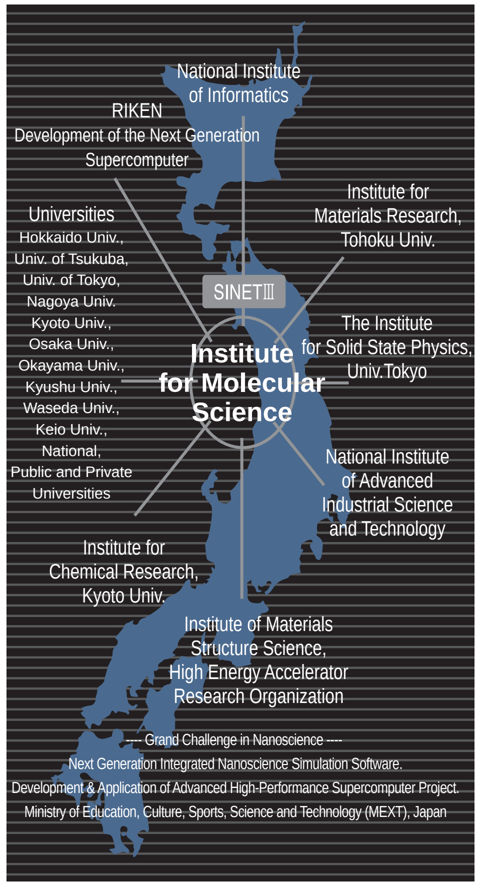


Drag Delivery System (Molecular Dynamics of Micelles)

Next Generation Energy



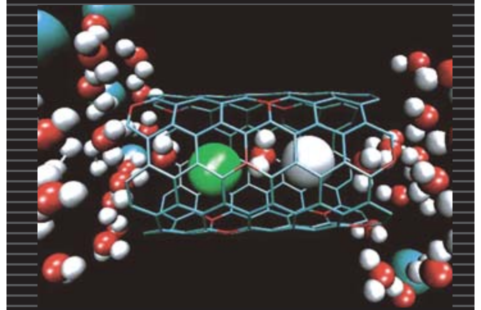
3D distribution of water around protein (Detected by 3D-RISM)



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

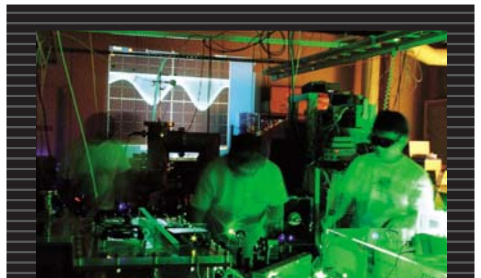
This project aims to establish a core computational science base for molecular and material systems and the development of methodologies for advanced calculations. The project has been organized by five institutes within the National Institutes of Natural Sciences, i.e. Institute for Molecular Science, 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.



Ion permeation in a mode channel.

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.



Experiment on Attosecond Coherent Control.

300kV Transmission Electron Microscopy.

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 Japanese 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 (920 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 nanobiotechnology field that is highly efficient in this joint project.

Inter-University Network for Efficient Utilization of Chemical Research Equipments

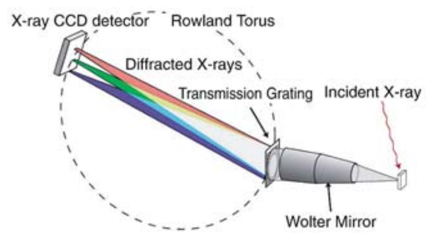
Academic and industrial activities in Chemistry in Japan have been highly influential over the past 30 years. Needless to say, it is highly important to improve the supporting environment for research and education in science and engineering. In particular, research equipments advances all the time to 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.

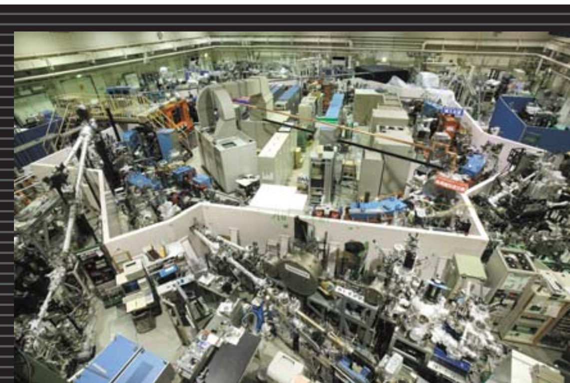
On April 7th 2007, the selected representatives from 72 universities gathered in Okazaki and decided to start the Inter-University Network for Efficient Utilization of Chemical Research Equipments. This system is operated through internet machine-time reservation and charging system by the help of equipment 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.





UVSOR Facility.

Next generation soft X-ray emission spectrometer developed at UVSOR.

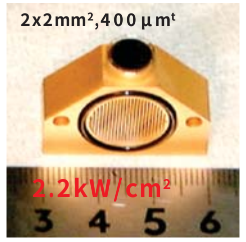
Research Center for Molecular Scale Nanoscience

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 offers public usage of the advanced ultrahigh magnetic field NMR (Nuclear Magnetic Resonance, 920 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.

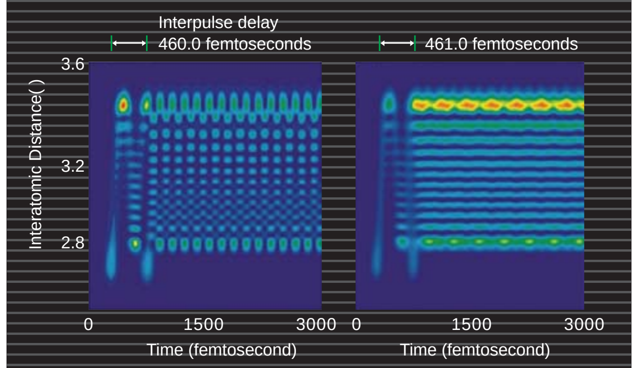
920 MHz NMR Spectrometer.

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 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) novel quantum-control schemes based on intense and ultrafast lasers; and (3) high-resolution optical imaging and nanometric microscopy. The center also serves as the core of the joint research project "Extreme Photonics" between IMS and RIKEN.



Microchip laser developed at the center.



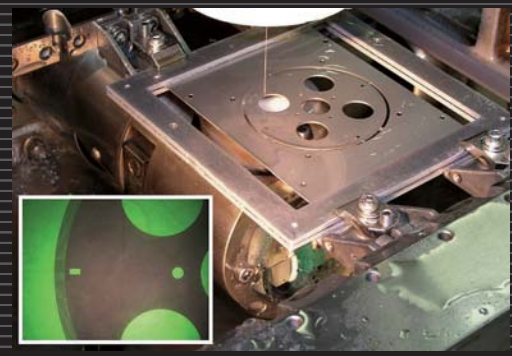
Theoretical simulation of quantum interferometric images generated in a single molecule with a pair of two laser pulses whose timing is controlled on the attosecond (10^{-18} sec) timescale.

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 in Yamate campus and ESR, SQUID magnetometer, powder and single-crystal 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.

CCD X-ray diffractometer.

Fluorescence spectrophotometer.



Machining a disk for selecting the supersonic molecular beam with a certain velocity by using a micro wire electric discharge machine.

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 Research Facilities

Super-High-Performance Molecular Simulator.

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.

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.

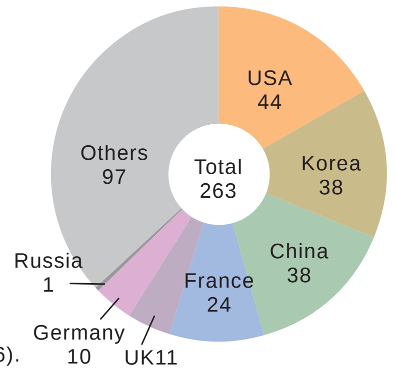
(6) Joint Studies Programs using beam lines of the UVSOR Facility.

(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 leading researchers through the collaboration and exchange among IMS and core Asian institutions: ICCAS (China), KAIST (Korea) and IAMS (Taiwan).



Visiting Foreign Researchers (2006).

Highly capable personnel nurtured by abundant research resources

Personnel Training : Education in Graduate School

IMS promotes pioneering and outstanding research by young scientists as a core academic organization in Japan. IMS trains graduate students in the Departments of Structural Molecular Science and Functional Molecular Science, Graduate School of Physical Sciences, the Graduate University for Advanced Studies (SOKENDAI). By virtue of open seminars in each research division, Colloquiums and the Molecular Science Forum to which speakers are invited from within Japan and all over the world, as well as other conferences held within IMS, graduate students have regular opportunities to be exposed to valuable information related to their own fields of research as well as other scientific fields. Graduate students can benefit from these liberal and academic circumstances, all of which are aimed at extending the frontiers of fundamental molecular science and to facilitate their potential to deliver outstanding scientific contributions.
For more details on the Departments of Structural Molecular Science and Functional Molecular Science, young scientists are encouraged to visit IMS through many opportunities such as the IMS Open Campus in May, Graduate-School Experience Program (Taiken Nyugaku) in August, Open Lectures in summer and winter, *etc*.

What is SOKENDAI?

The Graduate University for Advanced Studies (hereafter referred to by the Japanese contraction, "Sokendai") was founded in 1988 with the intention of cultivating new integrative research fields and to promote academic excellence through its doctoral course programs that 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.

SOKENDAI Hayama Campus

Common Facilities in Okazaki

Okazaki Library and Information Center

http://www.lib.orion.ac.jp/

In the Okazaki Library and Information Center, books and journals from three affiliated institutes (IMS, NIBB, NIPS) are collected, arranged and stored for the convenient use of staff and visiting users.
[Available services]
◎library is open 24 hours using ID cards
◎Online reading of journals and searches using Web of Science, SciFinder Scholar, *etc*.

Okazaki Conference Center

http://www.orion.ac.jp/occ-e/

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 (Daikaigi-shitsu), a middle room (Chu-kaigi-shitsu) and two small rooms (Sho-kaigi-shitsu) with seating capacities of 250, 150, and 50, respectively, are available.

Dormitories for Visiting Researchers

http://www.orion.ac.jp/occ-e/lodge/

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.

Administration

■Councillors

ESAKI, Nobuyoshi	Director, Institute for Chemical Research, Kyoto University
KATO, Shinichi	Chief Executive Officer, Toyota Central R&D Labs., Inc.
TSUCHIYA, Soji	Invited Professor, Faculty of Science, Josai University
NOGUCHI, Hiroshi	Culture News Editor, The Chunichi Shinbun Press
MILLER, H. William	Professor, University of California, Barkeley
LAUBEREAU, Alfred	Professor, Technische Universität München

■Research Consultants

HIROTA, Noboru	Professor Emeritus, Kyoto University
KONDOW, Tamotsu	Visiting Professor, Toyota Technological Institute
TAMAO, Kohei	Director, RIKEN Frontier Research System

■Advisory Committee

AWAGA, Kunio	Professor, Research Center for Materials Science, Nagoya University
ENOKI, Toshiaki	Professor, Graduate School of Science and Engineering, Tokyo Institute of Technology
FUJITA, Makoto	Professor, Graduate School of Engineering, The University of Tokyo
KATO, Masako	Professor, Graduate School of Science, Hokkaido University
MAEKAWA, Sadamichi	Professor, Institute for Materials Research, Tohoku University
NAKAJIMA, Atsushi	Professor, Faculty of Science and Technology, Keio University
SEKIYA, Hiroshi	Professor, Graduate Faculty of Sciences, Kyushu University
TANAKA, Kenichirou	Professor, Graduate School of Science, Hiroshima University (Vice chair)
TERAZIMA, Masahide	Professor, Graduate School of Science, Kyoto University
YAMASHITA, Kouichi	Professor, Graduate School of Engineering, The University of Tokyo
HIRATA, Fumio	Professor, Institute for Molecular Science
KOSUGI, Nobuhiro	Professor, Institute for Molecular Science
NAGASE, Shigeru	Professor, Institute for Molecular Science
NISHI, Nobuyuki	Professor, Institute for Molecular Science
OGAWA, Takuji	Professor, Institute for Molecular Science
OKAMOTO, Hiromi	Professor, Institute for Molecular Science
OHMORI, Kenji	Professor, Institute for Molecular Science
TANAKA, Koji	Professor, Institute for Molecular Science
URISU, Tsuneo	Professor, Institute for Molecular Science
YAKUSHI, Kyuya	Professor, Institute for Molecular Science (Chair)
YOKOYAMA, Toshihiko	Professor, Institute for Molecular Science

Personnel and Budget

Staff (as of April, 2007)

Director-General	1
Professors	15 (6)
Associate Professors	17 (8)
Assistant Professors	39
Technical Professers	37
Total	109 (14)

( ) Indicates the number of adjunct professors excluded.

Budget (2006) (Thousand yen)

Personnel	1,295,705
Research	1,859,207
Total	3,154,912

Grants-in-Aid (2006)* (Thousand yen)

Grant-in-Aid Scientific Research (KAKENHI, MEXT and JSPS)**	395,364
Joint Research	40,832
CREST, PRESTO, others(JST)**	32,500
Special Coordination Funds for Promoting Science and Technology from MEXT**	509,507
Others**	21,000
Total	999,203

* Included in the left table ** Including indirect expenses
MEXT : Ministry of Education, Culture, Sports, Science and Technology
JSPS : Japan Society for the Promotion of Science
J S T : Japan Science and Technology Agency