NATIONAL INSTITUTES OF NATURAL SCIENCES
Institute for Molecular Science
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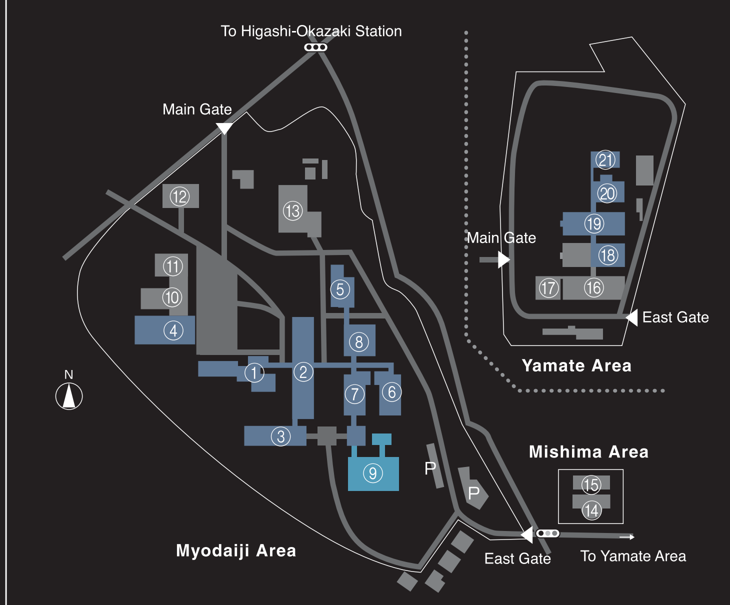
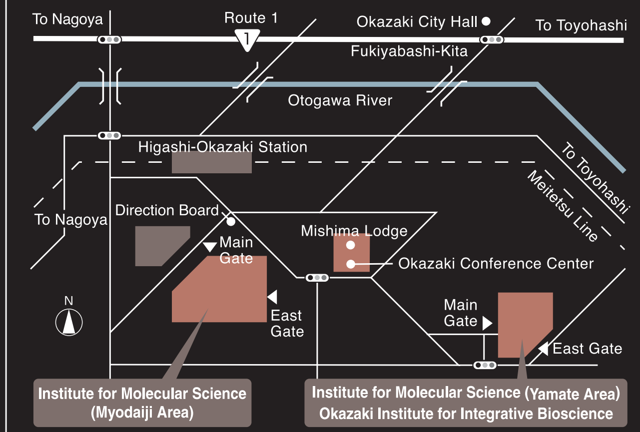
Phone: +81-564-55-7000 FAX: +81-564-54-2254
http://www.ims.ac.jp/

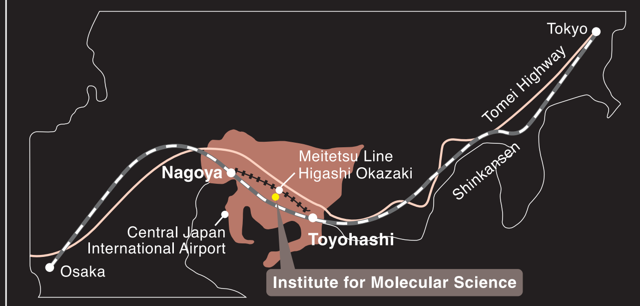
Campus Map



		(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.

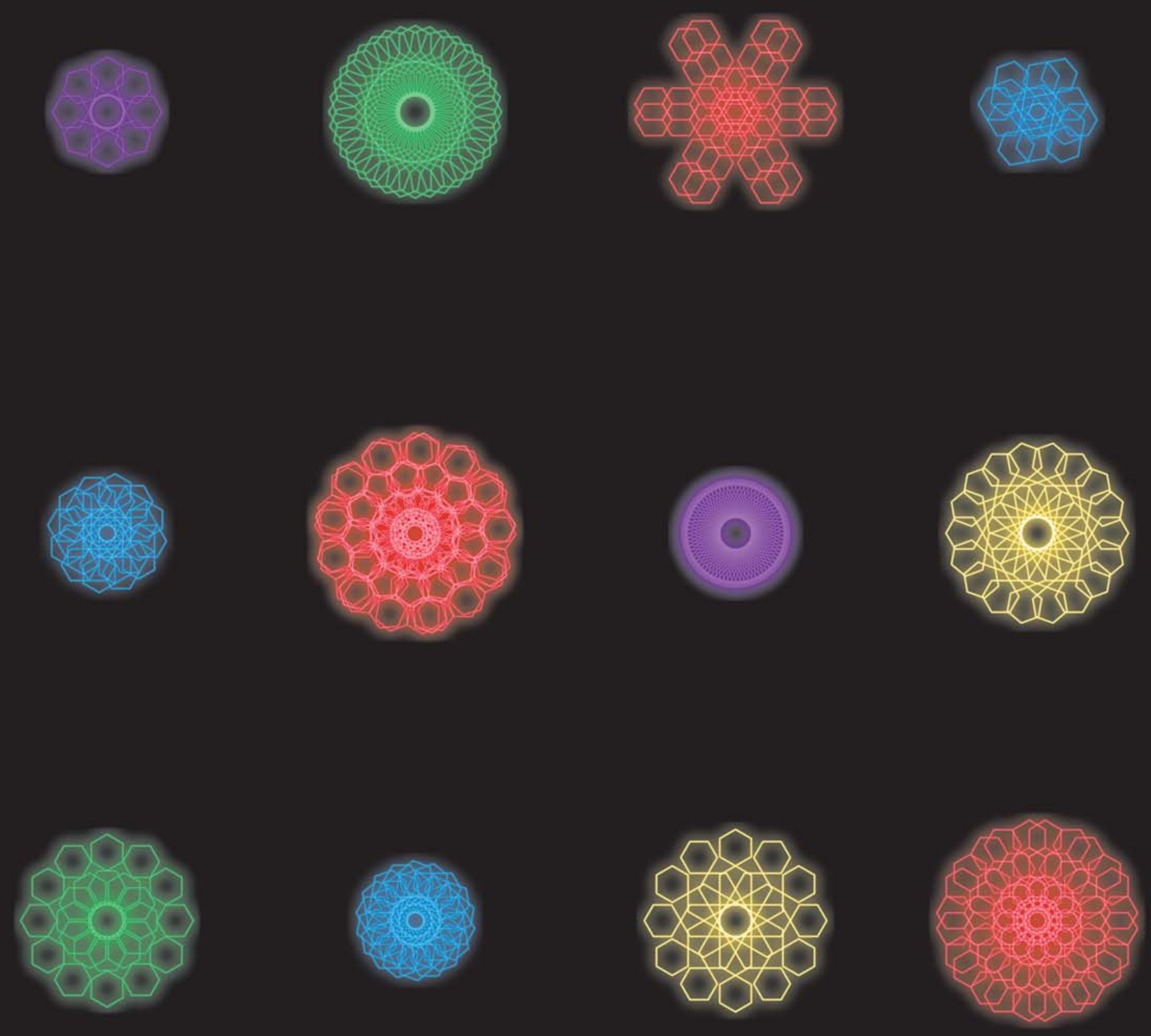
By Car

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).

2008.7

NATIONAL INSTITUTES OF NATURAL SCIENCES

IMS [Institute for Molecular Science]



2008

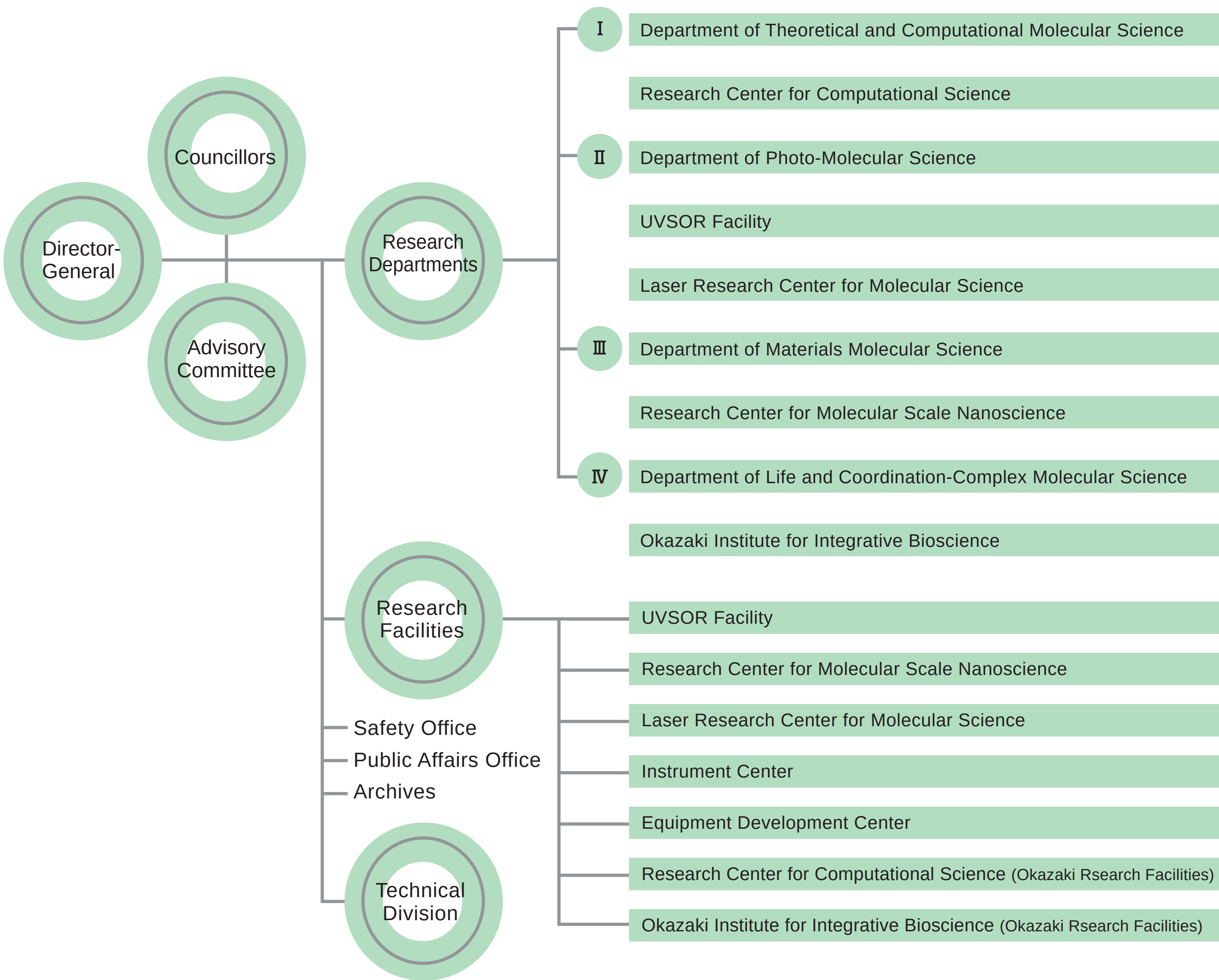
Unraveling the mysteries of molecules and extending their possibilities

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.

We have entered the fifth year of incorporation (privatization), and the evaluation of the first mid-term plan has started on a full-scale. As exemplified by this kind of a bit too much evaluation work and the fatigue of faculty members due to this, Japanese academic policy is still quite serious. It would be necessary to seriously reconsider the present system from the view-point of a permanent national policy. The development of science and culture is fundamental and very crucial for Japan to be an advanced cultural country.
The nationwide network system for efficient use of research equipments in chemistry, which has been constructed in order to prevent the collapse of the basis of scientific research in Japan with the participation of 72 national universities, is still financially poorly supported. However, we further work hard to make this system a solid one. In future it would be necessary to build up a much more stable budgetary framework than just a request from one institution. We believe that this kind of network system should be effective in other fields of science and is very economical and useful even in the case that the government budget becomes much healthier.
The special programs for the operation of which IMS is taking a major responsibility have been carried out nicely. (i) The nanotechnology network project has started satisfactorily to provide various facilities and supports to researchers. (ii) In the Asian Core Program, not only a variety of collaborative researches are going well, but also various activities to stimulate young scientists are regularly performed. (iii) The grand challenge to next-generation integrated nano-science in the next-generation supercomputer project has entered into a full-scale activity stage.
In the 2007 fiscal year, we carried out evaluation of all research groups and research facilities, and the results will be published in IMS Report 2007. Concerning the operation and management of IMS, we had discussions also inside the institute and some improvements are under investigation.
Considering the present national policy that tends to incline to the technological innovation and the short-sighted research projects, we, scientists, should keep appealing the significance of promotion of science and culture as a permanent national policy, and at the same time we should strive to pursue basic scientific researches of high quality and originality. As I always say, we should devote to that by pursuing the consciousness of truth, good and beauty , and furthermore the consciousness of myoh (妙) higher than the former.

April, 2008
NAKAMURA, Hiroki
Message from IMS Director-General

[ORGANIZATION]
Institute for Molecular Science



Organization

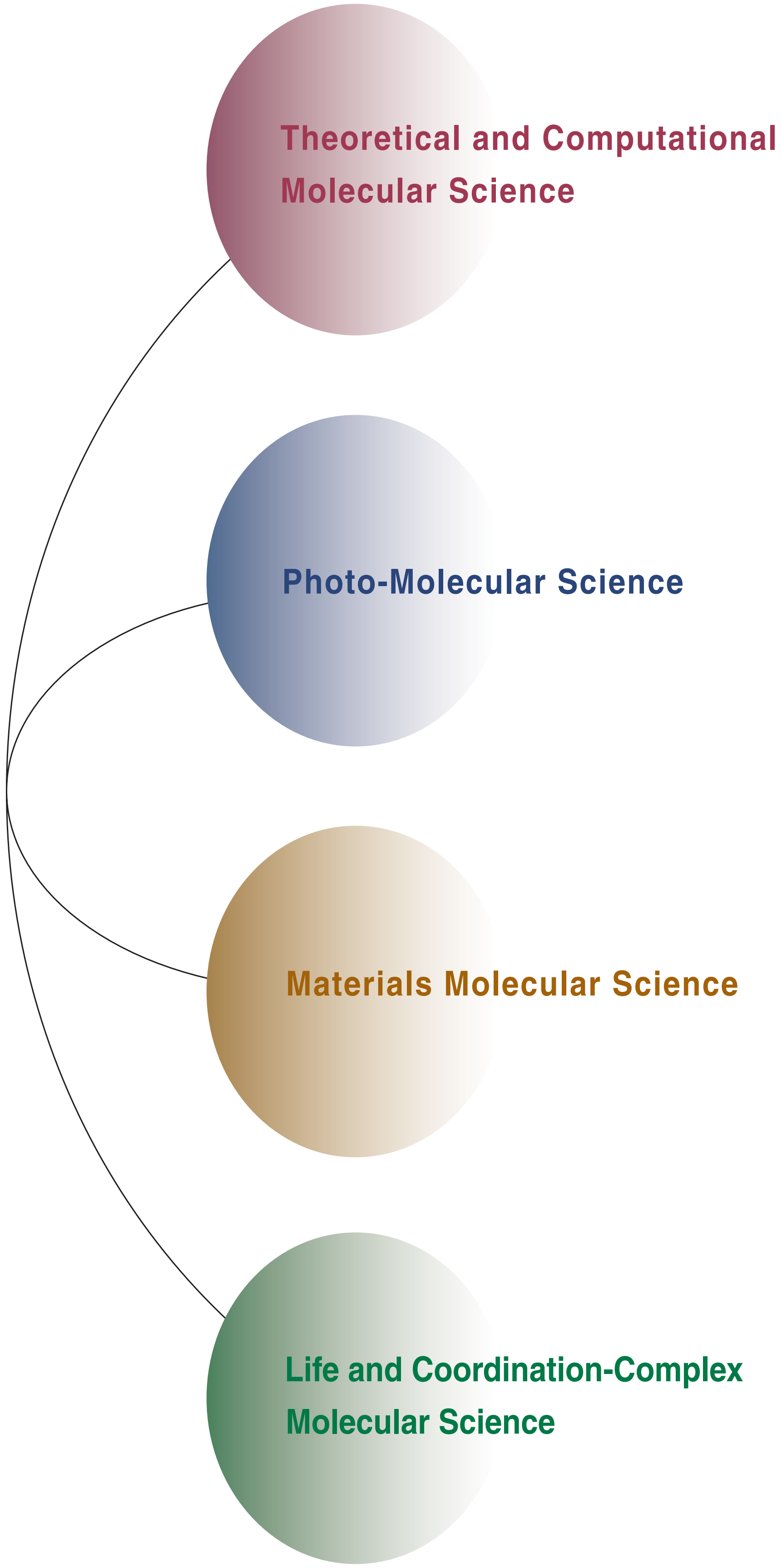
Research groups at the Institute for Molecular Science belong to Departments or Research Facilities. Technical groups primarily belong to one of the research facilities and have been responsible for energy conservation, safety, security, the information network, public affairs, and other such functions, 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(-March 2004)
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

Institute for Molecular Science

The research conducted by the Institute for Molecular Science (IMS) is broadly divided into four fields: theoretical and computational molecular science, photo-molecular science, materials molecular science, and life and coordination-complex molecular science. In each field, independent research groups led by professors are conducting most advanced researches based on the creative thinking of researchers. In addition, IMS is making efforts at promoting molecular science on a global basis by providing many researchers in Japan and abroad with collaborative research opportunities using its state-of-the-art facilities and forming a close-knit research partnership network with research centers in East Asia.



Theoretical and Computational Molecular Science

Describing invisible and intricate molecules

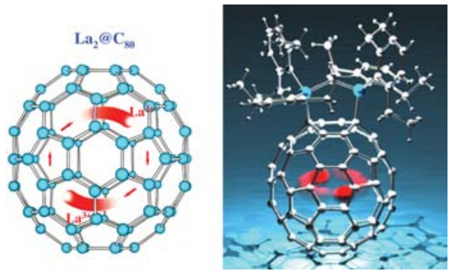
It is our ultimate goal to develop theoretical and computational methodologies that include quantum mechanics, statistical mechanics, and molecular simulations in order to understand the structures and functions of molecules in gasses and condensed phases, as well as in bio and nano systems.

Theoretical Molecular Science I

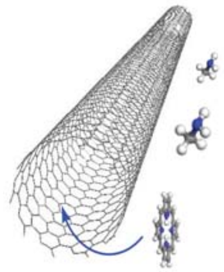
Theoretical Study and Design of Functional Molecules

NAGASE, Shigeru (Professor) mail:nagase@ims.ac.jp

In theoretical and computational chemistry, it is an important goal to develop functional molecules prior to or in cooperation with experiment. Thus, new bonds, structures and reactions provided by heavier atoms are investigated. In addition, chemical modification and doping of cage-like large molecules and clusters such as fullerenes and carbon nanotubes are investigated to develop functional nanomolecular systems. Efficient computational methods are also developed to perform reliable quantum chemistry calculations for large molecular systems.



Control of rotational motion by chemical modification and application to molecular devices.



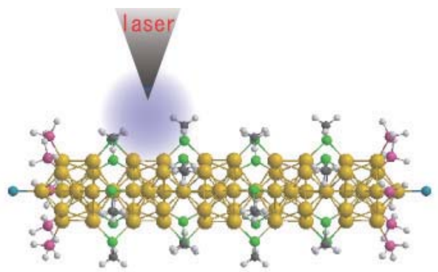
Functionalization by doping.

Theoretical Molecular Science I

Theory of Photoinduced Quantum Dynamics in Nanostructures

NOBUSADA, Katsuyuki (Associate Professor) mail:nobusada@ims.ac.jp http://raphael.ims.ac.jp/sub_index_E.html

All of the compounds in nature consist of a huge number of atoms and/or molecules. Nanometer-sized molecules, which are constructed from several tens to several hundreds of atoms, have characteristic geometrical and electronic structures, and unprecedented functions. Despite scientific interest in and technological importance of the nanometer-sized molecules, the fundamental properties of the molecules have not been well elucidated. We are currently investigating the photoinduced quantum (electron, spin, exciton) dynamics in various types of nanometer-sized molecules.



Schematic Diagram of Space Resolved Detection of a Nanostructure.

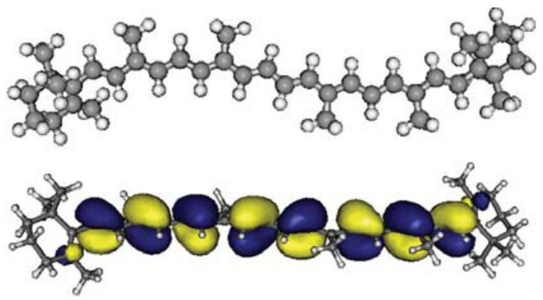
Theoretical and Computational Molecular Science

Theoretical Molecular Science I

Advanced Electronic Structure Theory for Predictive Quantum Chemistry

YANAI, Takeshi (Associate Professor) mail:yanait@ims.ac.jp

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 accurate 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.

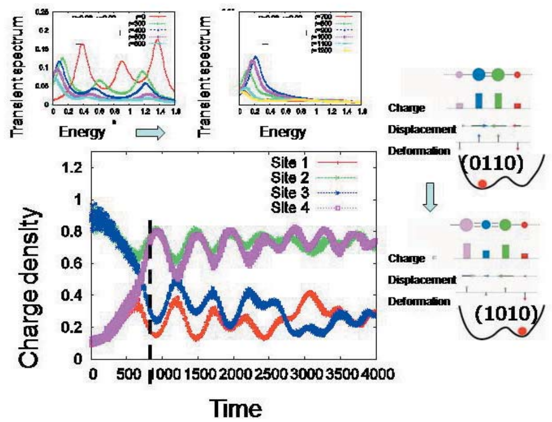


Molecular structure and molecular orbital of § carotene.

Theoretical Molecular Science II

Photoinduced Phase Transitions in Molecular Materials

YONEMITSU, Kenji (Associate Professor) mail:kxy@ims.ac.jp http://magellan.ims.ac.jp/index-0.htm



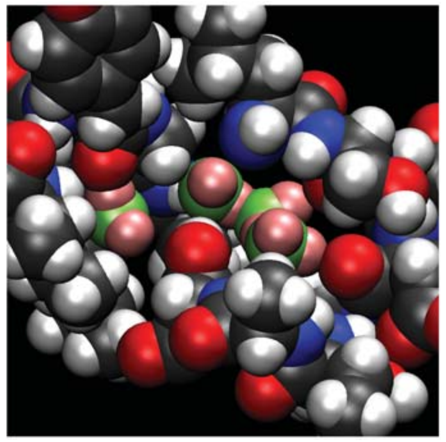
Photoinduced Change in Charge Order Pattern in $(EDO\text{-}TTF)_2PF_6$.

By theoretically clarifying how photoirradiation alters the properties of materials, we are able to control or rapidly switch the dielectric and/or transport properties of a material. Molecular Materials have characteristic directions with respect to the motion of their electrons and molecular arrangements can easily be modified. With the help of cooperativity between interacting electrons, a photoinduced phase transition in which the physical properties are macroscopically modified by very weak laser light can be achieved.

Theoretical Molecular Science II

Water Molecules Inside Protein, Detected by a Statistical Mechanics

HIRATA, Fumio (Professor) mail:hirata@ims.ac.jp http://daisy.ims.ac.jp/



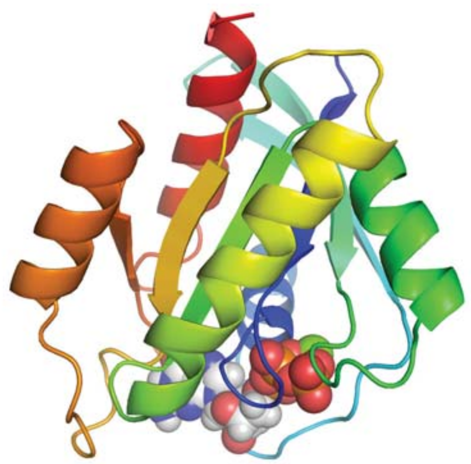
Water molecules inside protein (3D-RISM).

Most of proteins have internal cavities in which water molecules and other chemical compounds are trapped. Those molecules play essential roles as proteins perform their functions. For example, the reaction to produce sugar from cellulose is a hydrolysis in which water is directly involved in a chemical species. In that case, water and cellulose should be accommodated inside a protein cavity for the reaction to be taken place. Some of those water molecules have been detected by the X-ray crystallography. Recently, we have succeeded to detect such water molecules for the first time by mean of the statistical mechanics theory. The method can be readily extended to the problems such as the recognition of a ligand by a protein.

Computational Molecular Science

Theoretical Studies on Dynamics and Spectroscopies in Condensed Phases

SAITO, Shinji (Professor) mail:shinji@ims.ac.jp http://dyna.ims.ac.jp/index.html



Small G-protein Ras involved in cell proliferation.

Dynamics in condensed phases, e.g. liquids and biological systems, cause structural changes and chemical reactions over a wide range of time and spatial scales, and produce various properties and functions. Knowledge of temporal and spatial inhomogeneous dynamics is required to understand the chemical reactions and condensed phase dynamics. We have been investigating the dynamics of liquids and supercooled liquids and the hydrolysis in a G-protein, Ras, which is involved in the cell proliferation, by using molecular dynamics simulation and electronic structure calculation. In addition, we have been theoretically analyzing the intermolecular dynamics in terms of multi-dimensional spectroscopies.

Photo-Molecular Science

Create, observe and control with light

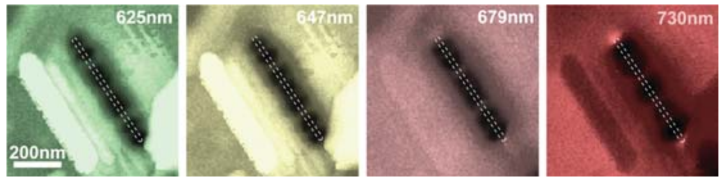
Molecules respond to photon irradiation in a variety of ways, including photo-induced transitions and photochemical reactions.
We have employed various light sources to elucidate molecular structures and properties and to control chemical reactions and molecular functions.
We have slso developed new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

Photo-Molecular Science I

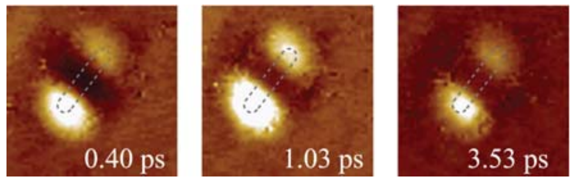
Exploring Nanomaterials by Novel Optical Microscopes

OKAMOTO, Hiromi (Professor) mail:aho@ims.ac.jp

It is impossible to resolve extremely small structures with a conventional optical microscope because of the diffraction limit (ca. 0.5 m for visible light). However, using recently developed near-field optical microscopy, we can observe nanometer-sized materials. This method makes it possible to take color photographs (i.e., spectral information) of nanomaterials. In addition, we can observe dynamic behaviors point-by-point on nanomaterials at the femtosecond timescale. We also found that wave function, which is essential in determining the material characteristics, is observable in some of nanomaterials. Based on such a methodology, we are currently conducting basic research into the novel optical properties and optical control of nanomaterials.



Near-field optical image of a nanometer-sized (length 510nm) metal rod. Wave function is visualized and is dependent on the wavelength observed.

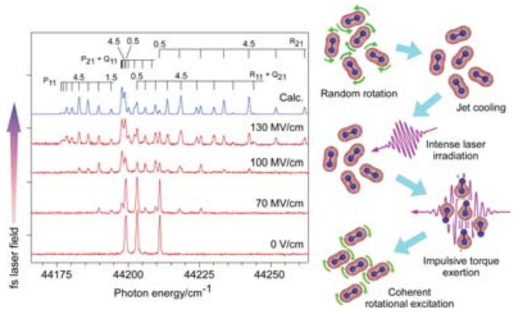


Images of ultrafast dynamic behavior of a nanometer-sized (length 300nm) metal rod. 1ps = 1000fs = 1/1,000,000,000,000s.

Photo-Molecular Science I

Quantum-State Manipulation of Molecular Motions

OHSHIMA, Yasuhiro (Professor) mail:ohshima@ims.ac.jp



Spectra of the NO molecule, excited to higher rotational states by the interaction with an intense ultrafast laser pulse, and the cartoon representing motions of molecules during the excitation process.

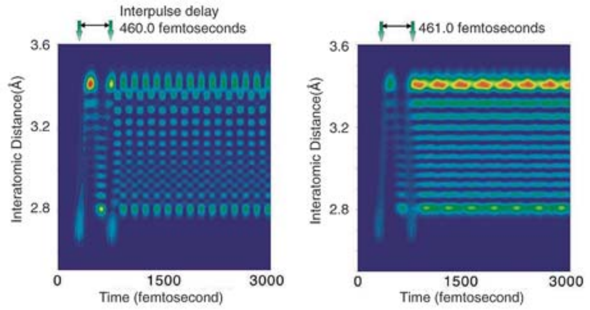
Molecules in gas phase undergo translational, rotational and vibrational motions in a random manner, and the total molecular system is a statistical ensemble that contains a number of molecules in many different states of motions. This research group aims to establish methods to manipulate the quantum-state distribution pertinent to molecular motions, by utilizing the coherent interaction with laser lights. Here lasers with ultimate resolution in time and energy domains are employed complementally and cooperatively for manipulation of molecular motions. At the present stage, the following subjects have been extensively explored: 1) an exploit of impulsive interaction with ultrafast intense laser fields to achieve a nonadiabatic excitation of molecular rotation, 2) realization of complete population transfer via an adiabatic interaction with coherent light fields from high-resolution ns pulsed laser systems, which have been newly constructed in this laboratory.

Photo-Molecular Science II

Attosecond Quantum Engineering

OHMORI, Kenji (Professor) mail:ohmori@ims.ac.jp

The wave nature of matter is at the heart of the quantum world. Quantum mechanics was founded more than 70 years ago, and our modern civilized societies are deeply indebted to inventions made possible by quantum mechanics such as computers and CD players. The quantum world is, however, not yet fully understood, and considerable potential for its application still exists. We are trying to control completely the wave nature of atoms and molecules with light to better understand the quantum world. Improved understanding of the quantum world will result in the development of novel quantum technologies such as single-molecule information processing and subnanoscale bond-selective chemistry.

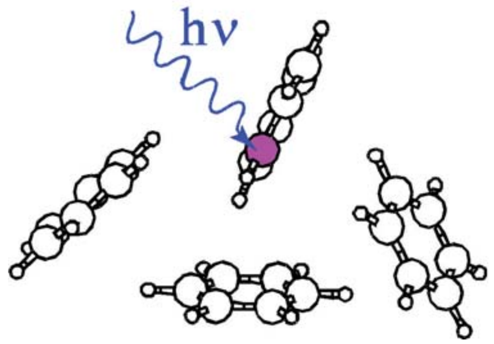


Theoretical simulation of quantum interferometric images generated in a single molecule with a pair of two laser pulses whose timing is controlled on the attosecond (10^{-18} sec) timescale.

Photo-Molecular Science III

Molecular Inner-Shell Spectroscopy

KOSUGI, Nobuhiro (Professor) mail:kosugi@ims.ac.jp



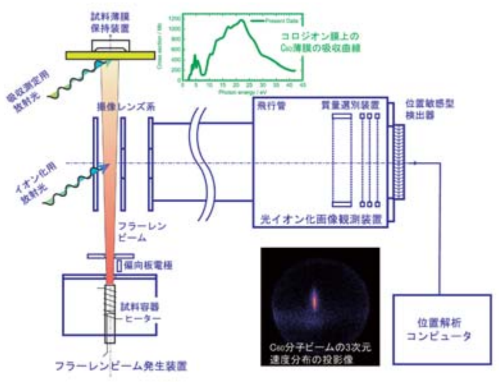
Site-selective inner-shell excitations in molecular clusters.

Inner-shell spectroscopy is applied to the molecular system, such as molecular clusters and molecular solids, by using soft X-rays from the undulator beamlines at the UVSOR synchrotron radiation facility. Unoccupied states in the system are revealed from inner-shell excitation by soft X-ray absorption. The inner-shell electron is strongly bound by an atom in the system but is slightly affected by surrounding atoms and chemical bonds. We can select inner-shell electron in each atom in molecules by choosing slightly different X-ray energies, and therefore know each atomic component in the unoccupied state in the system. Based on this characteristic, we are developing molecular inner-shell spectroscopy to reveal local electronic structures determining various kinds of interesting molecular properties.

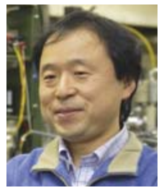
Photo-Molecular Science III

Photoionization and Photodissociation Dynamics in the Extreme UV

MITSUKE, Koichiro (Associate Professor) mail:mitsuke@ims.ac.jp http://www.ims.ac.jp/organization/mitsuke_g/



Apparatuses developed by our group for the velocity map imaging of C_{60} molecular beam and extreme UV photoabsorption of C_{60} thin film. In 2008 data from these machines were published for the first time.



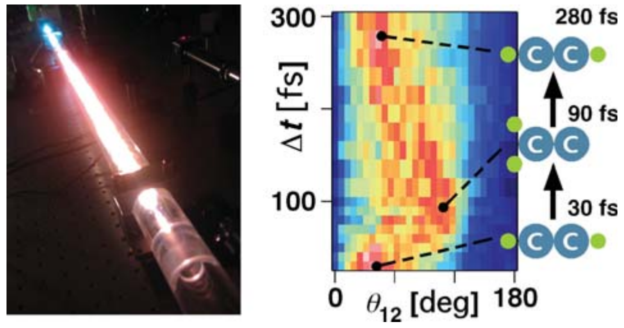
The main interests of our group focused on elementary reactions of solitary molecules induced by photoexcitation and/or photoionization in the extreme ultraviolet region ranging from 6nm to 200nm. Principal research subjects are (1) photoionization and photodissociation dynamics studied by electron and fluorescence spectroscopy, (2) development of high-resolution vacuum ultraviolet and soft-X ray monochromators for synchrotron radiation studies, (3) pump-probe or double resonance experiments combining synchrotron radiation and laser, and (4) photoionization and photodissociation mechanisms of fullerenes studied by quantitative photoabsorption spectroscopy, mass spectrometry together with theoretical analyses using the transient-state model, velocity-map imaging spectroscopy, and various coincidence techniques.

Photo-Molecular Science III

Molecular Dynamics in Intense Laser Fields

HISHIKAWA, Akiyoshi (Associate Professor) mail:hishi@ims.ac.jp http://groups.ims.ac.jp/organization/hishikawa_g/Welcome.html

Intense laser fields, comparable in magnitude with the Coulomb field within atoms and molecules, 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 cannot be observed in weak laser fields. We are seeking a deeper understanding of the behavior of molecules in intense laser fields to elucidate how molecules interact with light and to apply the new features they exhibit to the real-time visualization and the control of chemical reactions.



Generation of sub-10 fs ultrashort intense laser pulses (Left). Real-time visualization of intramolecular hydrogen migration by laser Coulomb explosion imaging (Right).

Advanced Accelerator Research

Light Source Developments by Using Relativistic Electron Beam

KATOH, Masahiro (Professor) mail:mkatoh@ims.ac.jp

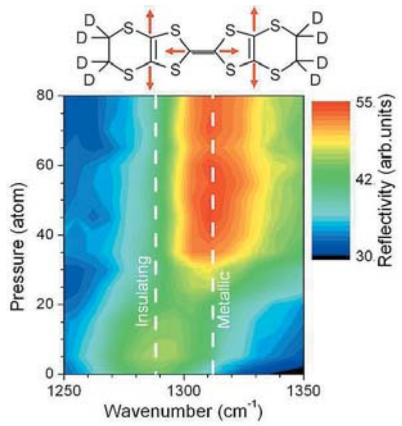
UVSOR-**II** at Institute for Molecular Science is an electron accelerator, which was constructed about 25 years ago. As the results of continuous efforts on improving the machine, its performance is in the world top level. Our research group is developing light source technologies by using the high quality electron beam from UVSOR-**II**, such as synchrotron radiation which is intense white light emitted by high energy electrons traveling in a strong magnetic field, free electron laser which is a laser technology based on synchrotron radiation and new technologies using laser-electron interactions. These lights are widely used in research works on molecular sciences and other research fields.

UVSOR-**II** Electron Storage Ring.

Advanced Solid State Physics

Investigation of the Functionality of Materials Using Synchrotron Radiation

KIMURA, Shin-ichi (Associate Professor) mail:kimura@ims.ac.jp http://www.uvsor.ims.ac.jp/staff/skimura/index.htm



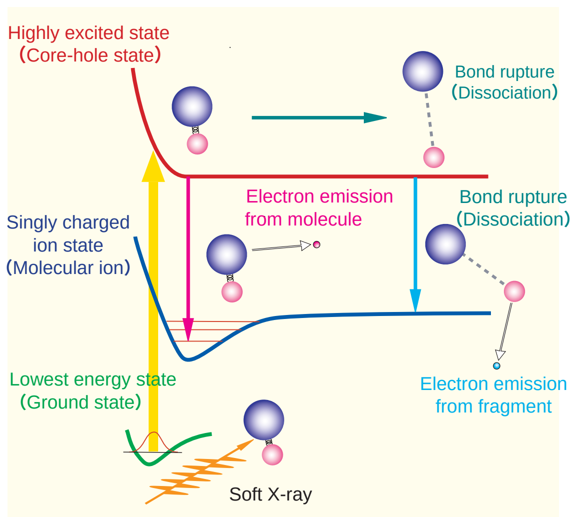
Pressure dependence of the molecular vibration mode due to the insulator-to-metal transition in an organic material.

Synchrotron radiation is a high brilliant light source with broad band from the terahertz to x-ray. The investigation of the functionality of materials under extreme conditions that has been regarded to be impossible up to now becomes available using the light sources. In particular, to clarify the origin of a metal-insulator transition under a high pressure, a high magnetic field and a low temperature provides important information for the design of functional materials based on electron correlations.

Advanced Photochemistry

Dynamical Processes Arising from Inner-Shell Hole Creation in Molecules

SHIGEMASA, Eiji (Associate Professor) mail:sigemasa@ims.ac.jp



A schematic representation of molecular core excitation and its subsequent decay processes.

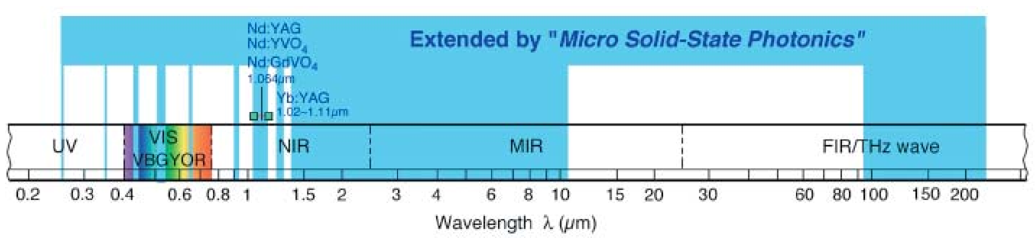
When a molecule is irradiated by high-energy radiation like X-rays, the inner-shell electron with no or very small contribution to any chemical bond in the molecule is excited. The molecule with an inner-shell vacancy thus created is quite unstable due to its fairly high internal energy, and subsequent electronic relaxation processes and/or ionic fragmentations take place. Such high-energy photochemical reactions strongly depend on which inner-shell electron in a molecule is involved, as well as the type of molecule. We inspect a wide variety of the reaction processes observed in each individual molecule by utilizing monochromatized synchrotron radiation, which is emitted by electrons orbiting in a storage ring.

Advanced Laser Development

Micro Solid-State Photonics

TAIRA, Takunori (Associate Professor) mail:taira@ims.ac.jp

"Micro Solid-State Photonics," based on the micro domain structure and boundary controlled materials, opens new horizon in the laser science. The engineered materials of micro and/or microchip solid-state, ceramic and single-crystal, lasers can provide excellent spatial mode quality and narrow linewidths with enough power. High-brightness nature of these lasers has allowed efficient wavelength extension by nonlinear frequency conversion, UV to THz wave generation. Moreover, the quasi phase matching (QPM) is an attractive technique for compensating phase velocity dispersion in frequency conversion. The future may herald new photonics.



Wavelength extension by Micro Solid-State Photonics.

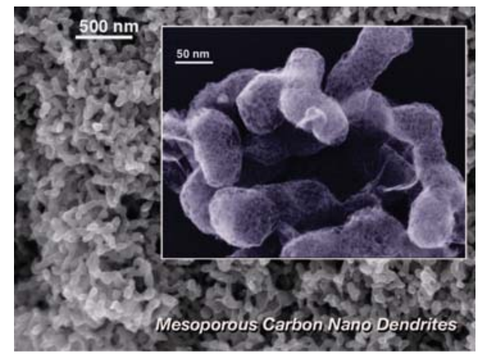
Materials development, functional control and developping new measurement techniques

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.

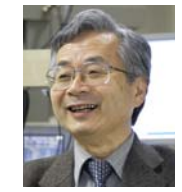
Electronic Structure

Functional Nano-Structures Produced from Metal Acetylides

NISHI, Nobuyuki (Professor) mail:nishi@ims.ac.jp http://nishi-group.ims.ac.jp/index_e.html



Mesoporous Carbon Nano-Dendrites with a BET surface of 1500 m^2/g.

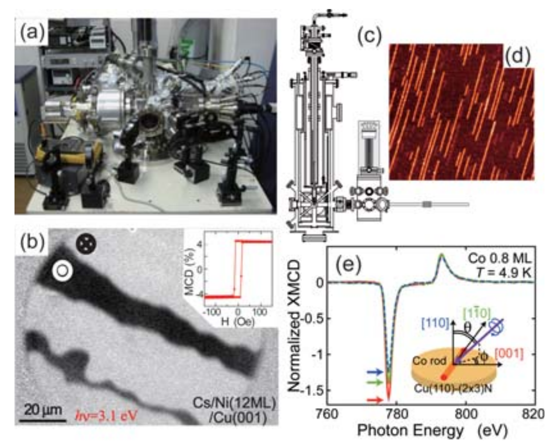


Metal acetylides composed of a carbon molecule (C≡C) unit and metal atom(s) generate nano-structures by the photo- or thermal-segregation reactions with various functions characteristic of metal species such as Schotoky Barrier devices, antirust transition metal nanomagnets, quasi-one-dimensional metal particle arrays, conductive nanosheets, oxygen sensors, hydrometers, and carbon nanodendrite electrodes. Mesoporous Carbon Nano-Dendrites simply produced from Ag_2C_2 exhibit BET surface areas as wide as 1500m^2/g and the surface is composed of graphen-type double wall or triple walls. They can be used as electrodes of super capacitors, Lithium Ion Batteries, and fuel cells.

Electronic Structure

Characterization of Magnetic Thin Films Using Photons

YOKOYAMA, Toshihiko (Professor) mail:yokoyama@ims.ac.jp http://msmd.ims.ac.jp/yokoyama_g/index_e.html



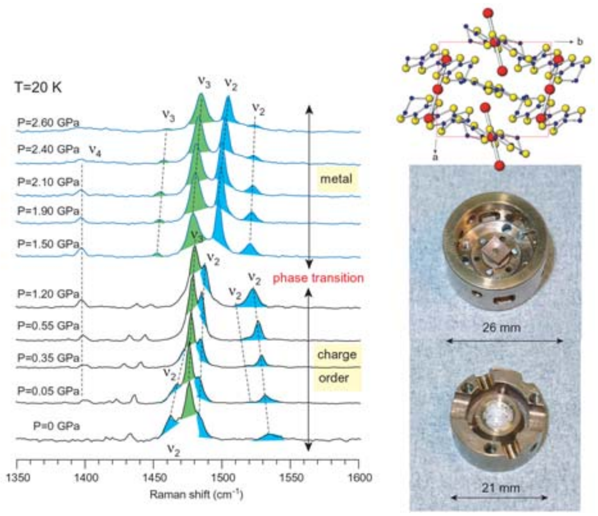
(a) Ultraviolet magnetic circular dichroism photoelectron emission microscope (UV MCD PEEM).
(b) First UV MCD PEEM image. The sample is 12 monolayer Ni on Cu(001) and shows upward and downward magnetic domains clearly.
(c) X-ray magnetic circular dichroism (XMCD) system with a superconducting magnet and a liq. He cryostat.
(d) STM image of Co nano-rods grown on Cu(001)-(2x3)N.
(e) Angle dependent XMCD spectra of the Co nanorods. The rods are likely to be magnetized perpendicularly to the rod axis within the substrate surface plane.

We investigate magnetic properties of surfaces and thin films mainly using photons. Recently, we exploited a substantially new magnetic microscope of magnetic circular dichroism photoelectron emission microscopy using ultraviolet lights and successfully obtained magnetic images of metal thin films. This method allows us to observe magnetic images with much higher spatial resolution than optical magnetic microscope, to perform in-laboratory measurements without using third-generation synchrotron radiation, and to investigate ultrafast spin dynamics using femtosecond lasers. Moreover, in our synchrotron radiation facility UVSOR-**II**, we constructed an X-ray magnetic circular dichroism system with a superconducting magnet (7tesla) and a liquid He cryostat (5K), and provide the apparatus for public usage for domestic and foreign researchers.

Electronic Properties

Observation of the Electronic Phase by Raman Spectroscopy

YAKUSHI, Kyuya (Professor) mail:yakushi@ims.ac.jp



Pressure dependence of the Raman spectrum of an organic conductor at 20 K. 1 GPa corresponds to 104 bar. This compound changes into metallic state above 1.5 GPa. Right figure shows a tool to generate high-pressure.

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.

Electronic Properties

Electronic Properties Investigation of Molecular Conductors by Magnetic Resonance

NAKAMURA, Toshikazu (Associate Professor) mail:t-nk@ims.ac.jp http://naka-w.ims.ac.jp/indexe.html

We investigate anomalous electronic phases observed in molecular-based conductors by magnetic resonance measurements such as NMR and ESR. Although pristine organic materials are well-know as insulators, we can get electric conductors after electro chemical carrier doping. The fundamental properties of molecular-based conductors have been clarified. However it is also true that a lot of unsolved problems remain. Moreover, molecular-based conductors attract much attentions by their possible functionality because of various electronic phases. Magnetic resonance is advanced technique which enables us to clarify character of materials by nuclear and/or electron magnets as probes without contact and destruction.

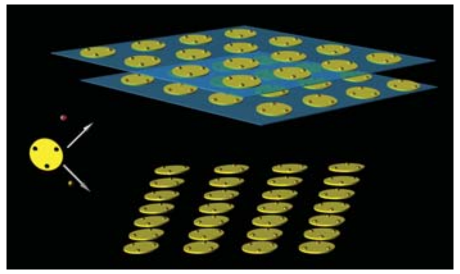
(Left) Pulsed FT-NMR Spectrometer, (Right) Multi-frequency pulsed-ESR Spectrometer, Bruker E680.

Molecular Functions

Function Design of Supramolecules and Macromolecules

JIANG, Donglin (Associate Professor) mail:jiang@ims.ac.jp

How to control the composition, the alignment, and the cooperativeness of molecules is a key issue in function design of supramolecules and macromolecules. This laboratory focuses on novel extended „-electronic systems, with a challenge to function design of intelligent photo, electronic, and spin functional supramolecules and macromolecules that are responsive to external stimuli, through chemical construction based on a protocol that seamlessly fuses molecular design, precise integration, and function exploration. We develop spin functional supramolecules with photo-controllable spin state and magnetism, by taking advantage of spatially confined alignment of metallo-complexes. We explore conjugated gigantic macromolecules with 2-D extended sheet structure and create unprecedented functional macromolecules with tunable nanopores.



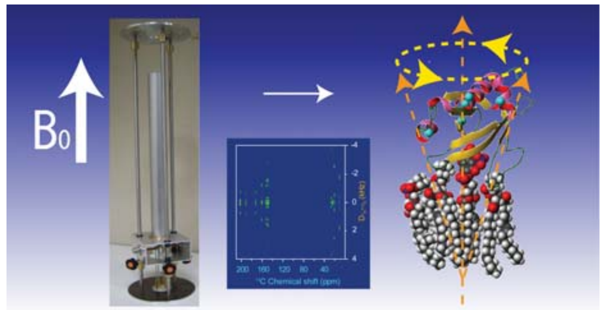
Tuning of nanostructures by metal ions.

Molecular Functions

Methodology Developments of Solid State NMR for Biomolecules

NISHIMURA, Katsuyuki (Associate Professor) mail:nishimur@ims.ac.jp

Atomic nuclei of molecules have nuclear spin, which placed in magnetic field behave as small magnet, and it is possible to control those behaviors by applying electromagnetic waves at suitable frequency. This technique is referred to as nuclear magnetic resonance (NMR), and it enables to determine interatomic distances and interbond angles accurately without damage of molecules. Many of important biomolecules such as membrane proteins, and advanced materials are insoluble and functional at amorphous state. Thus solid state NMR is essential for the characterization of those molecules. We are mainly working on the methodology and hardware developments for solid state NMR and its applications.



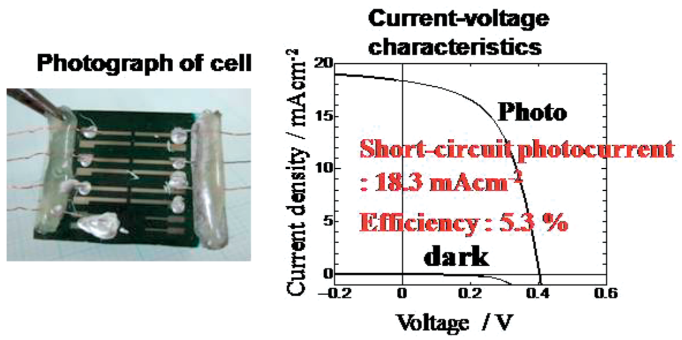
(Left) The developed solid state NMR probe and 2D NMR spectrum.
(Right) Dynamics of peripheral membrane protein bound to lipid bilayers.

Molecular Nanoscience

Organic Electronic Devices

HIRAMOTO, Masahiro (Professor) mail:hiramoto@ims.ac.jp

Organic EL television was commercialized last year. Next target of organic electronics is organic solar cell. Our group accomplished the world record conversion efficiency of 5.3% based on the fundamental research on the organic semiconductors such as ultra-high purification, nanostructure design.

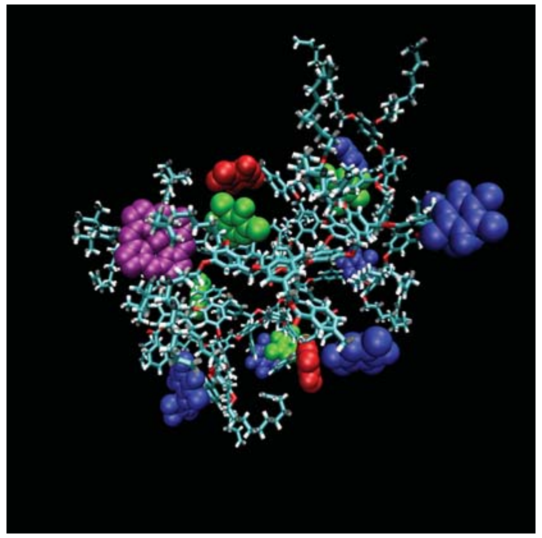


Organic semiconductor, organic solar cell, ultra-high purification, nanostructure design.

Molecular Nanoscience

Building Photosynthesis from Artificial Molecules

NAGATA, Toshi (Associate Professor) mail:toshi-n@ims.ac.jp



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

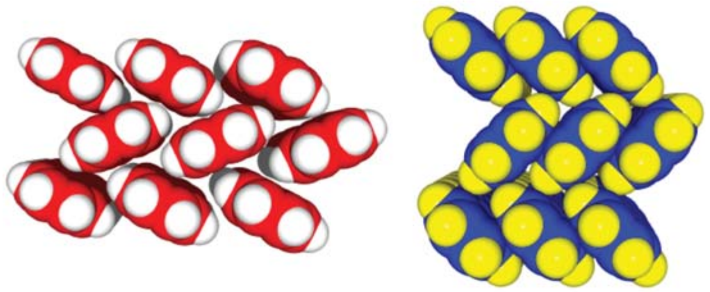
Photosynthesis supports all sorts of activities of lives on the earth, through conversion of solar energy to chemical energy. This is done by green plants by use of a set of complicated biological molecules, which constitute one of the finest piece of molecular machinery ever created by Nature. Our research aims at mimicking this machinery with artificial molecules. The ultimate goal is, like plant photosynthesis, to make useful organic compounds out of carbon dioxide with solar energy. Although this is still far away, we are confident that, by combining our knowledge on the mechanism of natural photosynthesis and our experience on synthetic chemistry, we will be able to realize a new form of photosynthesis of purely artificial origin.

Molecular Nanoscience

Synthesis of Organic Semiconductors and Application to Devices

SUZUKI, Toshiyasu (Associate Professor) mail:toshy@ims.ac.jp

Organic semiconductors are of great interest because of the applications for plastic electronics such as organic light-emitting diodes, transistors, and photovoltaics. Unlike conventional inorganic semiconductors, organic devices are thin and flexible. We have been synthesizing new organic semiconductors for such devices. Our collaborators construct the devices to see the performance of our materials. Some of them are used in the laboratories of universities and companies worldwide for science and technology.



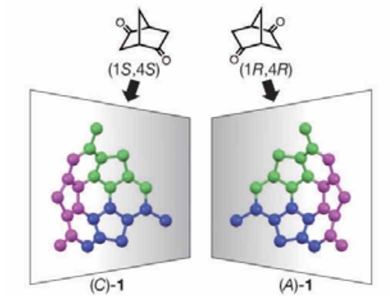
Crystal structures of pentacene and perfluoropentacene as the organic semiconductors.

Molecular Nanoscience

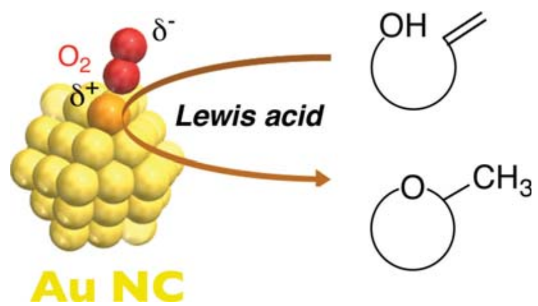
Science of Buckybowls and Development of Metal Nanocluster Catalyst

SAKURAI, Hidehiro (Associate Professor) mail:hsakurai@ims.ac.jp http://groups.ims.ac.jp/organization/sakurai_g/english/

Bowl-shaped „-conjugated compounds including partial structures of the fullerenes or the cap structure of nanotubes, which are called buckybowls, are of importance not only as model compounds of fullerenes but also as their own chemical and physical properties. However, very few buckybowls has been achieved for preparation mainly due to their strained structure. In addition, most of thus-reported procedures are performed under severe reaction conditions, limiting the sort of the introducible atoms/functional groups. In the present works, we develop the rational route to the various kinds of buckybowls using the organic synthesis approach. We are also interested in the development of metal nanocluster catalyst and its application to synthetic organic chemistry.



Synthesis of homochiral Buckybowls.



Unique catalytic activity of Gold nanoclusters.

Life and Coordination-Complex Molecular Science

Realizing vital functions and efficient chemical reactions

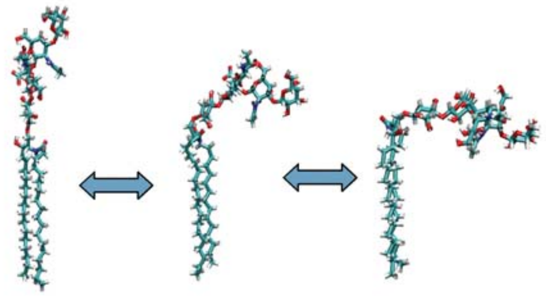
We are undertaking researches to elucidate the molecular mechanisms responsible for various biological functions and to develop new molecular devices using biological molecules. We are also working on energy-material conversion, organic molecules transformation in water, and activation of small inorganic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

Biomolecular Sensing

Developments of Neural Network Analyzer and Medical Molecular Science

URISU, Tsuneo (Professor) mail:urisu@ims.ac.jp http://groups.ims.ac.jp/organization/urisu_g/contact.html

The neurodegenerative diseases such as Alzheimer s disease are the real intractable disease, concerning which number of patients are more than several tens of million in the world and the number is still increasing, and both of the pathogenesis cause and the treatment methods are still unclarified. We consider that the analysis of the molecular structure and the function of the pathogen molecules in vivo in the biological system is essentially important to solve this problem. Defining these researches as medical molecular science a new field of the molecular science, we are developing neural network analyzer device, and carrying out the research to make clear the molecular structure of the pathogen relating molecules at the synapse. We are also analyzing the molecular structure and the dynamical behavior of the pathogen relating molecules in the well defined system of the lipid bilayer mimicking the cell membrane.

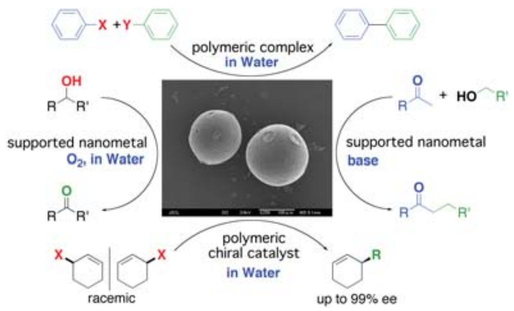


The reactivity of GM1 which locates on the synapse cell membrane changes significantly depending on its molecular structure.

Complex Catalysis

Development of Heterogeneous Catalysis toward Ideal Chemical Processes

UOZUMI, Yasuhiro (Professor) mail:uo@ims.ac.jp http://groups.ims.ac.jp/organization/uozumi_g/



Typical Examples of Heterogeneous Aquacatalyses using Amphiphilic Polymer-Supported Metal Complexes and Metal Nanoparticles: A typical SEM image of the polymeric catalyst (center); C-C bond forming catalysis (top); aerobic alcohol oxidation (left); α-alkylation with alcohol (right); asymmetric allylic substitution (bottom).

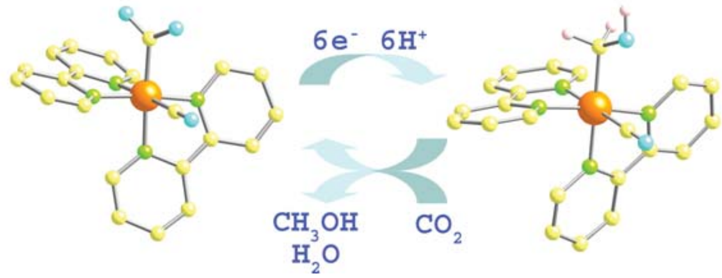
Our research interests lie in the development of transition metal-catalyzed reaction systems toward ideal (highly efficient, selective, green, safe, simple, etc.) organic transformation processes. In one active area of investigation, we are developing the heterogeneous aquacatalytic systems. Various 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.

Functional Coordination Chemistry

Development of Complex Catalyst Aimed at Reversible Conversion between Chemical and Electrical Energy

TANAKA, Koji (Professor) mail:ktanaka@ims.ac.jp

Construction of a new energy conversion system instead of thermal and nuclear power generation is one of the most important problem which now confronts scientists. We have been developing transition-metal complex catalysts for electro- and photochemical multi-electron reduction of CO_2 (fixation of electricity and solar energy) and electrochemical oxidation of organic compounds (regeneration of electricity) for the purpose of energy conversion between chemical energy and electricity. We have succeeded electrochemical conversion of CO_2 to CO on the ruthenium complex having polypyridyl ligands and generation of oxyl- and aminyl-radical complexes from the corresponding aqua and ammine complexes by pH gradient. These complexes have potential to catalyze multi-electron reduction of CO_2 and electrochemical oxidation of organic compounds, respectively.

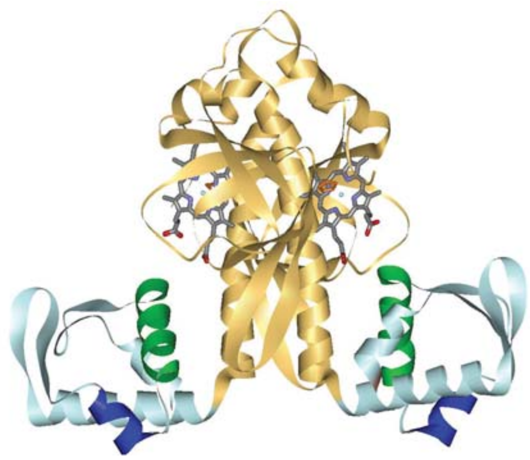


Multi-electron reduction of CO_2.

Biomolecular Functions

The Regulation of Biological Function by Metalloproteins

AONO, Shigetoshi (Professor) mail:aono@ims.ac.jp http://groups.ims.ac.jp/organization/aono_g/



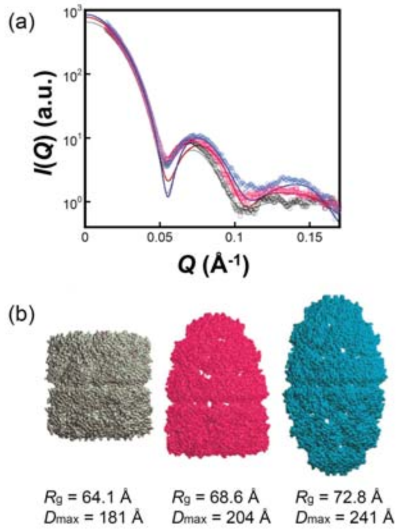
Structure of the CO-sensor protein containing an iron-porphyrin complex.

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.

Biomolecular Functions

Molecular Mechanisms of Protein Folding

KUWAJIMA, Kunihiro (Professor) mail:kuwajima@ims.ac.jp http://gagliano.ims.ac.jp/index-e.html



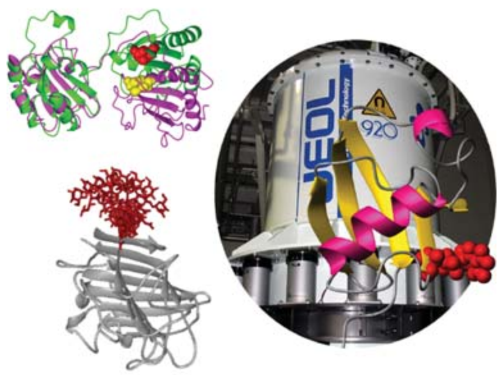
(a) Small-angle X-ray scattering patterns of molecular chaperones, GroEL and the GroEL-GroES complexes.
(b) The three-dimensional structures of GroEL (gray), the bullet-type GroEL-GroES complex (magenda), and the football-type GroEL-GroES complex (cyan)(Inobe et al., *Biophys. J.* 94: 1392-1402 (2008)).

How does a protein fold into its native functional three-dimensional structure from its one-dimensional amino acid sequence (= genetic information)? To elucidate such a problem of protein folding, we are studying (1) *in vitro* refolding reactions of model globular proteins, and (2) functional mechanisms of molecular chaperones that are known to mediate protein folding in biological cells. To this end, we are using various spectroscopic and biophysical techniques, including NMR, small-angle X-ray scattering and calorimetry, as well as molecular biological techniques such as site-directed mutagenesis.

Biomolecular Functions

Elucidation of Dynamical Structures of Biomolecules toward Understanding the Mechanisms Underlying Their Functions

KATO, Koichi (Professor) mail:kkatonmr@ims.ac.jp



Probing dynamics of biomacromolecules by NMR.

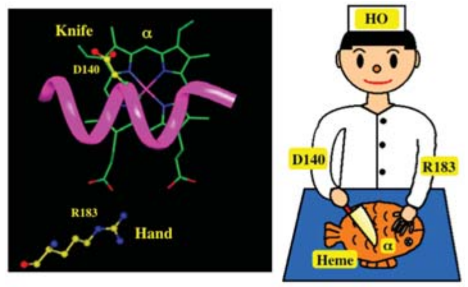
A wide variety of biomacromolecules have adopted their own three-dimensional structures during the long process of evolution and thereby enabled them to express sophisticated functions in the biological systems. Our biomolecular studies are based on detailed analyses of structures and dynamics of various biological macromolecules and their complexes at atomic level, primarily using nuclear magnetic resonance (NMR) spectroscopy. In particular, we conducted studies aimed at elucidating the dynamic structures of glycoconjugates and proteins for integrative understanding of the mechanisms underlying their biological functions. For this purpose, we use multidisciplinary approaches integrating the methodologies of molecular and cellular biology and nanoscience along with molecular spectroscopy.

Biomolecular Functions

Molecular Mechanism of Metalloenzymes

FUJII, Hiroshi (Associate Professor) mail:hiro@ims.ac.jp

Metalloenzymes are biologically important macromolecules, which catalyze various chemical reactions in vivo, such as hydrolysis, oxidation, reduction, and oxygenation. These diverse functions of metalloenzymes are thought to depend on ligands from amino acids, coordination structure, and protein structure in immediate vicinity of metal ions. However, it has not been still clear how each metalloenzyme controls its function. To answer the question, we are studying molecular mechanism of metalloenzyme with synthetic metalloenzyme model complexes and mutant enzymes.



Molecular mechamism of heme oxygenase.

Leading the sustainable future of Japan

— Grand Challenge in Nanoscience —

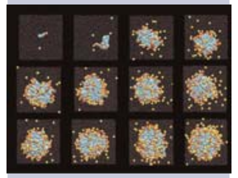
Next Generation Integrated Nanoscience Simulation Software Development & Application of Advanced High-Performance Supercomputer Project Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan

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 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.

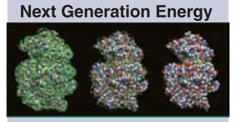
Next Generation Nano Information Function and Materials

Next Generation Nano Biomolecules

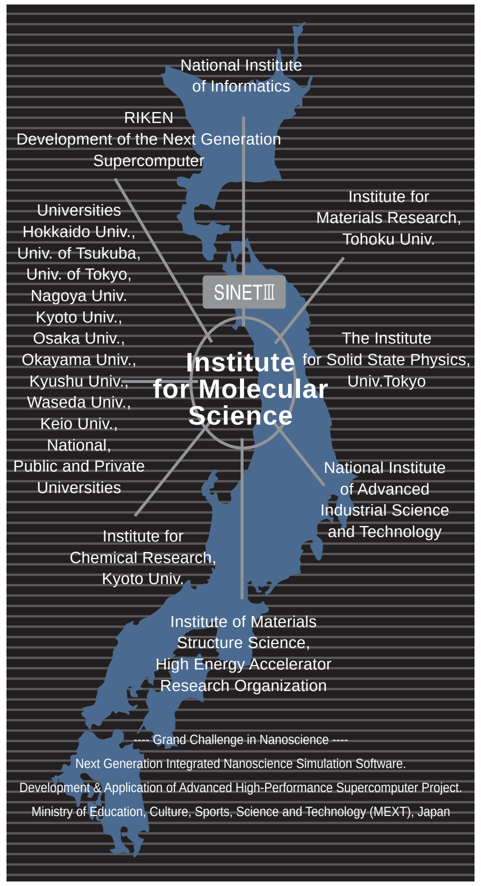


Drag Delivery System (Molecular Dynamics of Micelles)

Next Generation Energy



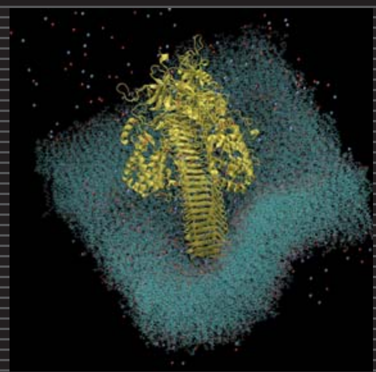
3D distribution of water around protein (Detected by 3D-RISM)



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

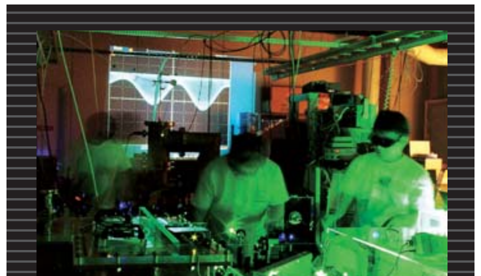
This project aims to establish a core computational science base for molecular and material systems and the development of methodologies for advanced calculations. The project has been organized by five institutes within the National Institutes of Natural Sciences, i.e. Institute for Molecular Science,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



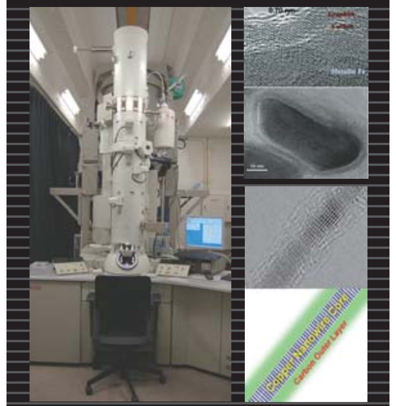
Massive molecular dynamics to simulate puncture of lipid bilayer by gp5.

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 (left), Fe nanoparticle embedded in graphite (right top), and Cu nanocable covered with carbon cube.

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 by university and government researchers but also by private company researchers. 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 supporting 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.

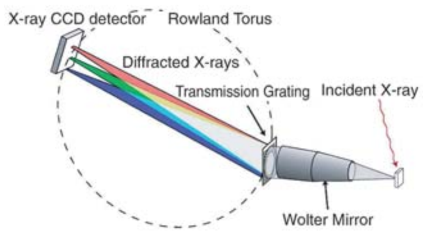
On April 7th 2007, the selected representatives from 72 universities gathered in Okazaki and decided to start the Inter-University Network for Efficient Utilization of Chemical Research Equipments. This system is operated through internet machine-time reservation and charging system by the help of equipment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

Research Facilities

UVSOR Facility

Vacuum ultraviolet (VUV) light is not alive when the solar light reaches the earth, because the VUV light strong interaction with molecules in the air . The wavelength of the VUV light is between ultraviolet (UV) light and X-rays. Since the VUV light is indispensable in photo-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.

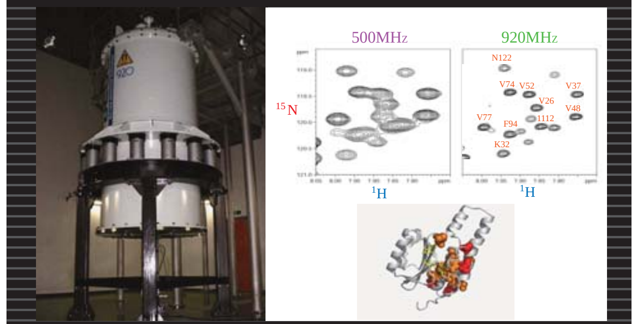


UVSOR Facility.

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

Research Center for Molecular Scale Nanoscience

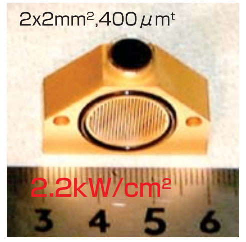
The Center was established in 2002 with the mission of undertaking comprehensive studies of “Molecular Scale Nanoscience.” The Center consists of one divisions staffed by full-time researchers and two divisions staffed by adjunctive researchers. Their mandates are 1) fabrication of new nanostructures 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.



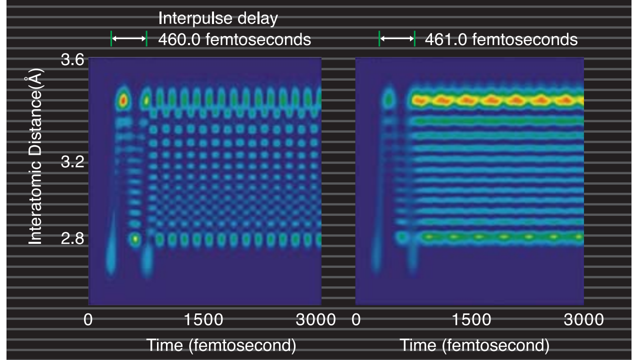
920 MHz NMR Spectrometer (left) and measured example (right).
Substantially higher resolution than the 500 MHz data is clearly demonstrated.

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.



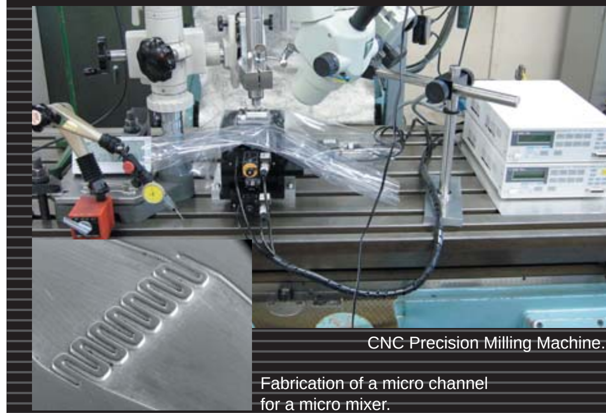
Theoretical simulation of quantum interferometric images generated in a single molecule with a pair of two laser pulses whose timing is controlled on the attosecond (10^{-18} sec) timescale.

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.



CNC Precision Milling Machine.

Fabrication of a micro channel for a micro mixer.

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.

Super-High-Performance Molecular Simulator.

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 was introduced further in this year to realize much higher computational environment.

Okazaki Institutes for Integrative Bioscience

The main purpose of the Okazaki Institute 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.

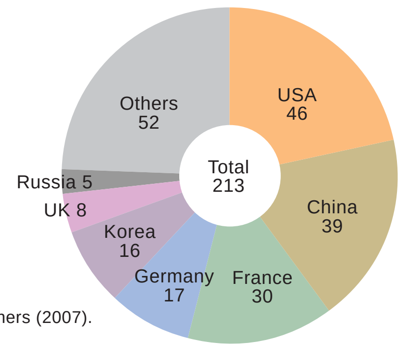
Serving as a core organization for domestic research

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 (2007).

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

TOKITOH, Norihiro	Director, Institute for Chemical Research, Kyoto University
KATO, Shinichi	Chief Executive Officer, Toyota Central R&D Labs., Inc.
TSUCHIYA, Soji	Professor Emeritus, Tokyo University
	Visiting Professor National Chiao Tung University
NOGUCHI, Hiroshi	Culture News Editor, The Chunichi Shinbun Press
MILLER, H. William	Professor, University of California, Barkeley
LAUBEREAU, Alfred	Professor, Technische Universitat München

■Research Consultants

HIROTA, Noboru	Professor Emeritus, Kyoto University
KONDOW, Tamotsu	Visiting Professor, Toyota Technological Institute
IRIE, Masahiro	Professor, Rikkyo University

■Advisory Committee

EBATA, Takayuki	Professor, Graduate School of Science, Hiroshima University
ENOKI, Toshiaki	Professor, Graduate School of Science and Engineering, Tokyo Institute of Technology
FUKE, Kiyokazu	Professor, Graduate School of Science, Kobe University (Vice chair)
KATO, Masako	Professor, Graduate School of Science, Hokkaido University
NAKAJIMA, Atsushi	Professor, Faculty of Science and Technology, Keio University
SEKIYA, Hiroshi	Professor, Graduate Faculty of Sciences, Kyushu University
SHINOHARA, Hisanori	Professor, Department of Chemistry / Inititute for Advanced Research, Nagoya University
WATANABE, Yoshihito	Professor, Research Center for Materials Science, Nagoya University
YAMASHITA, Kouichi	Professor, Graduate School of Engineering, The University of Tokyo
YAMASHITA, Masahiro	Professor, Graduate School of Science, Tohoku University
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
OHMORI, Kenji	Professor, Institute for Molecular Science
OKAMOTO, Hiromi	Professor, Institute for Molecular Science
TANAKA, Koji	Professor, Institute for Molecular Science
URISU, Tsuneo	Professor, Institute for Molecular Science(Chair)
YAKUSHI, Kyuya	Professor, Institute for Molecular Science
YOKOYAMA, Toshihiko	Professor, Institute for Molecular Science

Personnel and Budget

Staff (as of April, 2008)

Director-General	1
Professors	15 (10)
Associate Professors	14 (7)
Assistant Professors	38
Technical Professers	36
Total	104 (17)

( ) Indicates the number of adjunct professors excluded.

Budget (2007) (Thousand yen)

Personnel	1,230,465
Research	2,000,248
Total	3,230,713

Grants-in-Aid (2007)* (Thousand yen)

Grant-in-Aid Scientific Research (KAKENHI, MEXT and JSPS)**	334,258
Joint Research	26,371
CREST, PRESTO, others(JST)**	84,864
Special Coordination Funds for Promoting Science and Technology from MEXT**	590,576
Others**	29,006
Total	1,065,075

* Included in the left table ** Including contract-based research and 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