

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.



Molecular scientists, by carrying on a “dialog” with molecules, seek to ascertain the origin of diversity in natural phenomena. In doing so, they set for themselves an extremely wide range of research goals, from understanding the behavior of individual molecules to that of collective molecular processes on the scale of life forms and in space. The Institute for Molecular Science (IMS) is one of the world’s core research facilities for molecular science and is a center for inter-university joint research, as well. Since its foundation 35 years ago, the IMS, in addition to conducting groundbreaking research, has also fostered the development of many young scientists, who are now widely known in the fields of physics and chemistry.

Currently, the IMS is engaged in four areas of research: theoretical and computational molecular science, photo-molecular science, materials molecular science and life-and-coordination-complex molecular science. It operates seven research facilities, including the UVSOR synchrotron radiation

facility. The staff persons at IMS are making steady progress in basic research on molecular structures, reactions and functions demonstrating “novel molecular capabilities.”

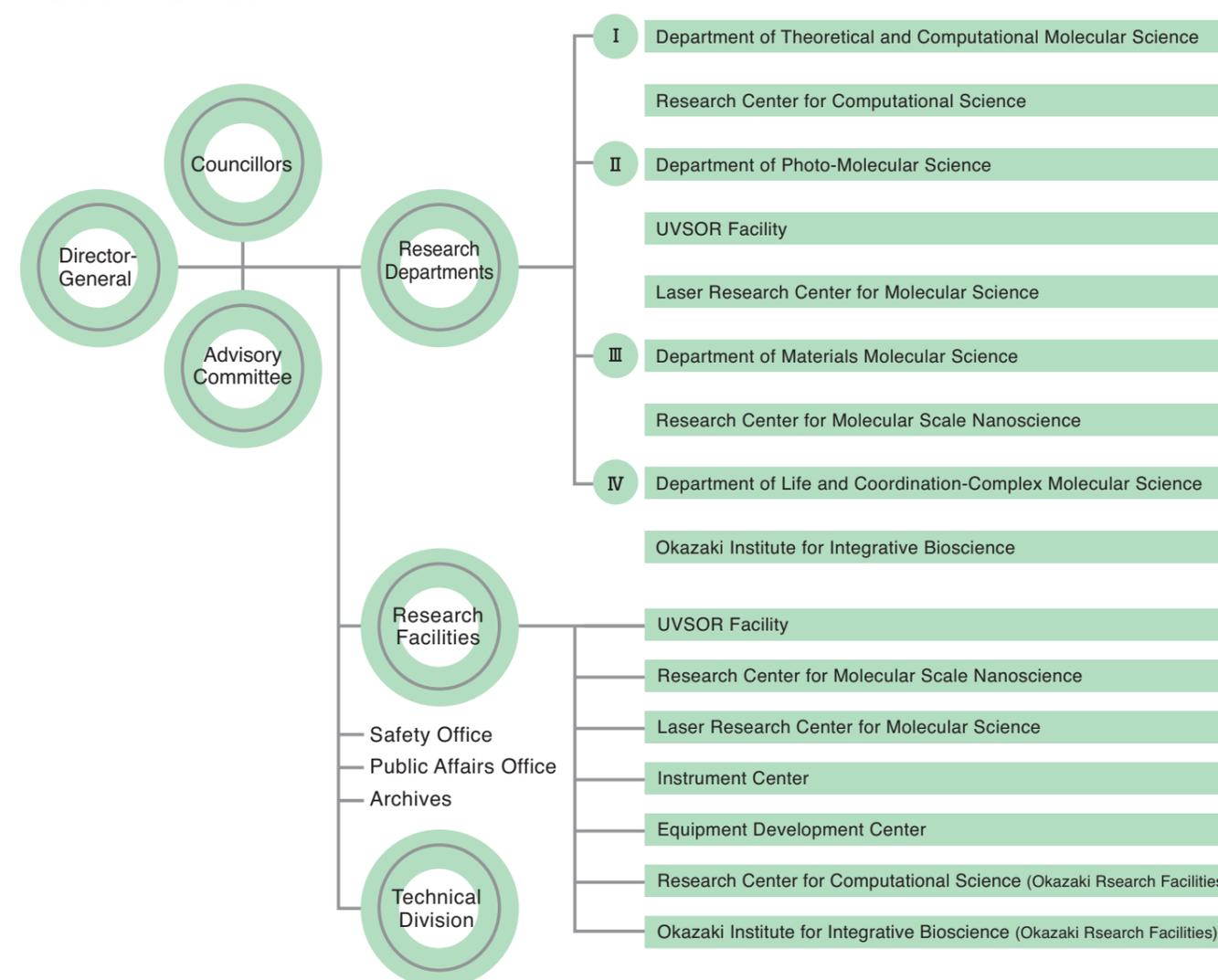
IMS researchers are now employing a new scientific perspective in order to examine the boundary between “micro” and “macro” phenomena, the so-called “post-nano” world, which is regarded as being “an intrinsic arena for the generation of life” and for the evolution of functioning molecular materials. In this “arena” various types of molecular groups interact with each other by exchanging energy, entropy and information. Clarifying the principles of the post-nano world is essential to understanding the “molecular wisdom” of Nature. Elucidation of these highly-configured molecular processes will no doubt impact considerably on many academic areas and lead to key innovations in the fields of energy, environment and information technology. This, in brief, is the “investigative adventure,” which the IMS is now carrying out for the future benefit of all people.

April, 2010

OHMINE, Iwao

Message from NINS, IMS Director-General

[ORGANIZATION] Institute for Molecular Science



● Organization

The Institute for Molecular Science is one of the inter-university research institutes of a unique model for national and international cooperative research systems. 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 Natural Sciences, which is one of the Inter-University Research Institute Corporations. 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 and research institutions in Japan and foreign countries. The nature of these joint research initiatives are beyond the framework of their respective universities and research institutes, and allows these researchers to 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

Photo-Molecular Science

Materials Molecular Science

Life and Coordination-Complex 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.

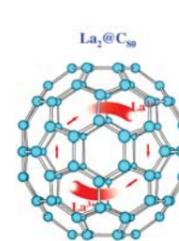
Theoretical Molecular Science I

Theoretical Study and Design of Functional Molecules

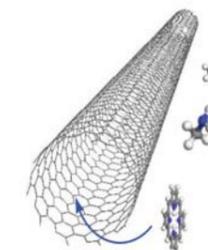
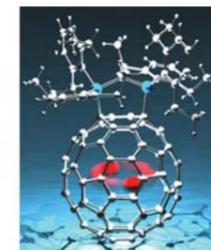
NAGASE, Shigeru (Professor)

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.

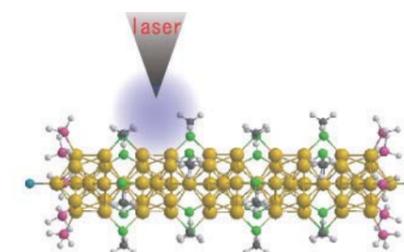
Theoretical Molecular Science I

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.

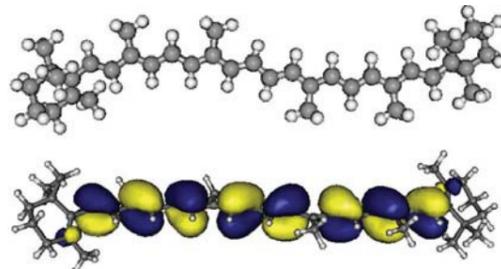
Theoretical Molecular Science I

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.



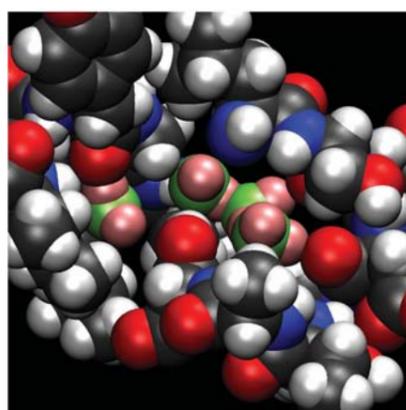
Molecular structure and molecular orbital of β carotene.

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.

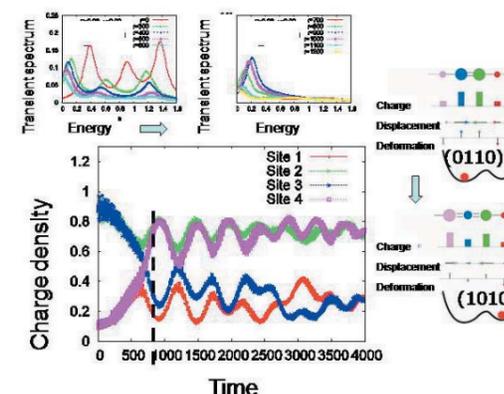


Theoretical Molecular Science II

Photoinduced Phase Transitions in Molecular Materials

YONEMITSU, Kenji (Associate Professor)

mail:kxy@ims.ac.jp http://magellan.ims.ac.jp/index-O.htm



Photoinduced Change in Charge Order Pattern in (EDO-TTF)₂PF₆.

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.

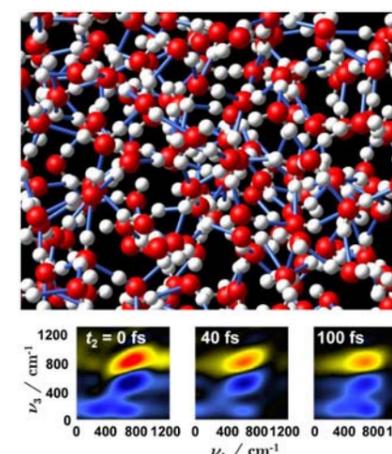


Computational Molecular Science

Theoretical Studies on Dynamics and Spectroscopies in Condensed Phases

SAITO, Shinji (Professor)

mail:shinji@ims.ac.jp http://dyna.ims.ac.jp/index.html



A snapshot of liquid water (upper) and time-dependence of two-dimensional IR spectroscopy of intermolecular motions in water calculated from molecular dynamics simulation (lower).

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.

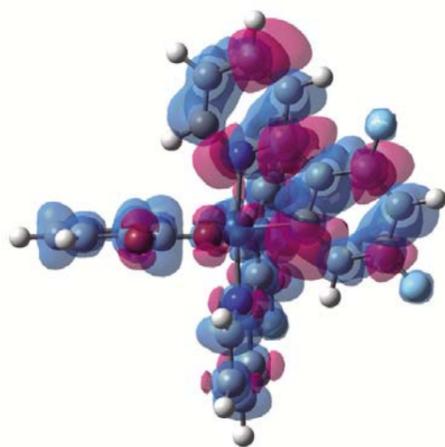


Computational Molecular Science

Exploring New Field of Theoretical Chemistry Based on Electronic Structure Theory

EHARA, Masahiro (Professor)

mail:ehara@ims.ac.jp



Electron density reorganization due to electronic excitation.

Wide varieties of chemical phenomena appear on the basis of the electronic structure of molecules. The purpose of our group is to clarify the "essence" of the chemical phenomena and to create "new chemical concept" using the electronic structure theory. We develop the highly accurate excited-state theory and apply it to molecular spectroscopy, photochemistry, and photo material science, etc. We also investigate the catalytic reactions and surface photochemistry.

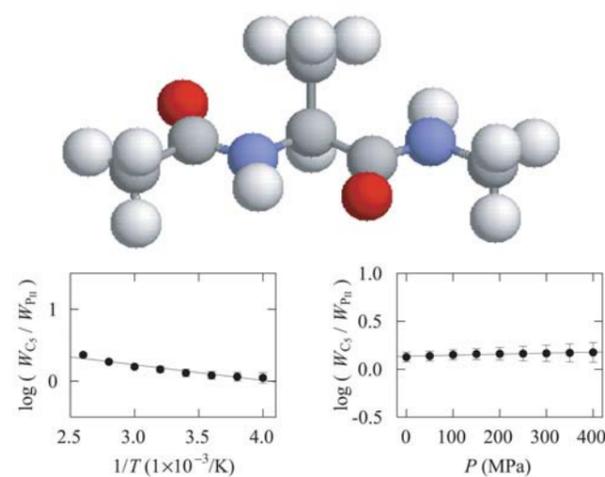


Computational Molecular Science

Simulations of Biomolecules under Extreme Conditions

OKUMURA, Hisashi (Associate Professor)

mail:hokumura@ims.ac.jp



Structure of an alanine dipeptide and its temperature and pressure dependences.

Molecular structures are changed under various conditions of temperature and pressure. It was, however, difficult so far to study theoretically these structural changes. I have recently proposed a powerful simulation algorithm to solve this problem. I have succeeded in calculating enthalpy and volume of each state of biomolecules accurately. I expect that this algorithm would be of great use for the theoretical analysis of biomolecules under various conditions of temperature and pressure.



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 also developed new and advanced light sources for molecular science.

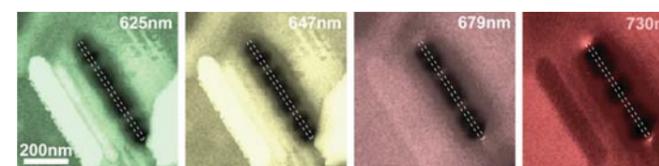
Photo-Molecular Science I

Exploring Nanomaterials by Novel Optical Microscopes

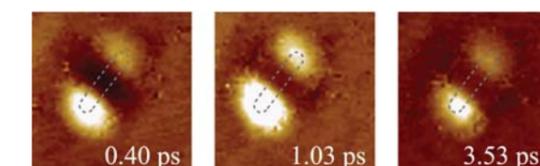
OKAMOTO, Hiromi (Professor)

mail:aho@ims.ac.jp

It is impossible to resolve extremely small structures with a conventional optical microscope because of the diffraction limit (ca. $0.5\mu\text{m}$ 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 images of a nanometer-sized (length 510nm) metal rod. "Wave function" is visualized and is dependent on the wavelength observed.



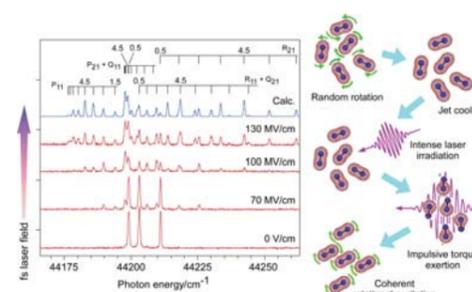
Images of ultrafast dynamic behavior of a nanometer-sized (length 300nm) metal rod. 1ps = 1000fs = 1/1,000,000,000,000s.

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 motions, 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.



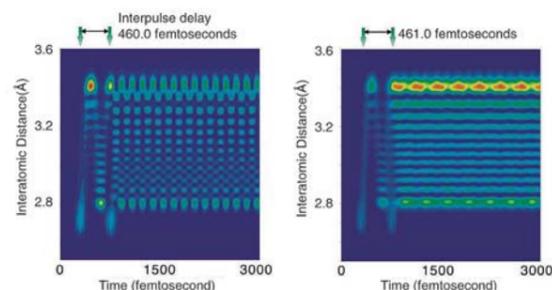
Photo-Molecular Science II

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.



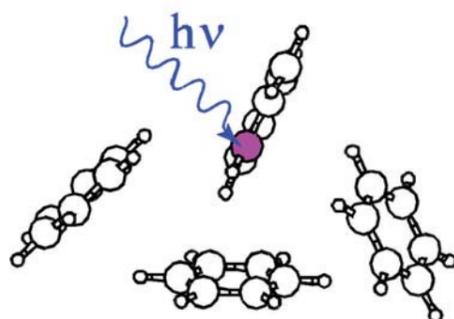
Theoretical simulation of quantum interferometric images generated in a single molecule with a pair of two laser pulses whose timing is controlled on the attosecond (10^{-18} sec) timescale.

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 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.

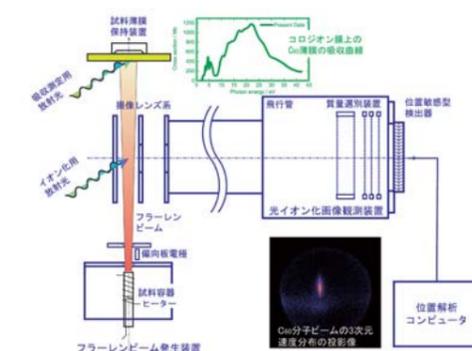


Photo-Molecular Science III

Photoionization and Photodissociation Dynamics in the Extreme UV

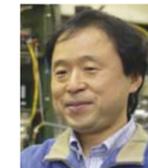
MITSUKE, Koichiro (Associate Professor)

mail:mitsuke@ims.ac.jp http://groups.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 are 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.



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.



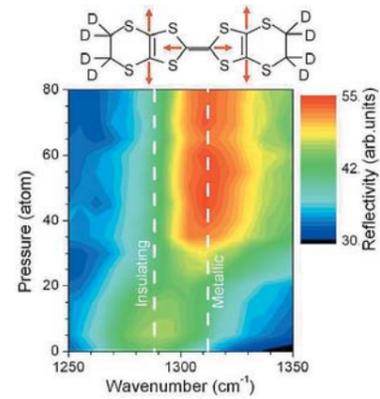
UVSOR-II Electron Storage Ring.



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.



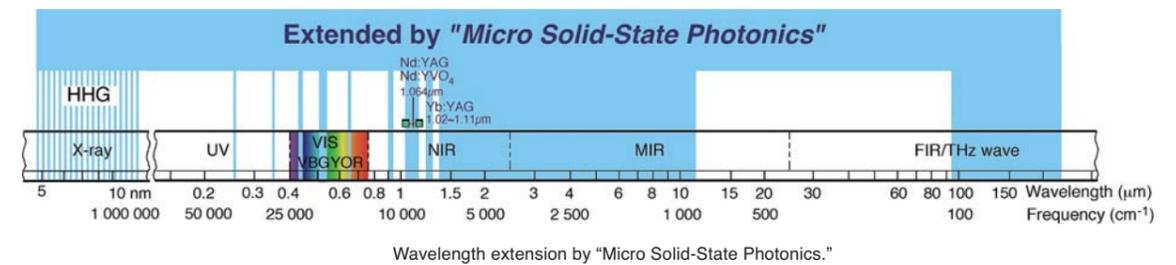
Advanced Laser Development

Micro Solid-State Photonics

TAIRA, Takunori (Associate Professor)

mail:taira@ims.ac.jp

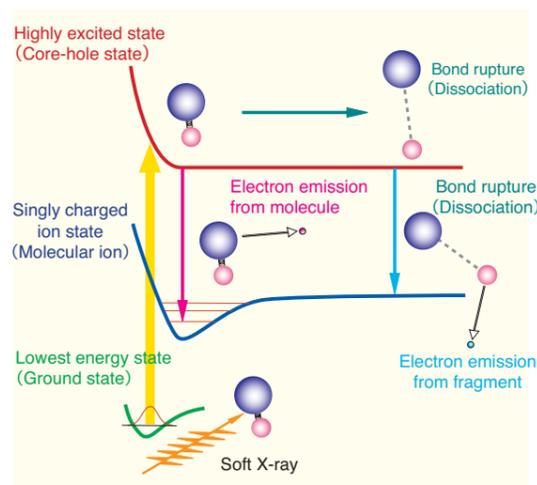
"Micro Solid-State Photonics," based on the micro domain structure and boundary controlled materials, opens new horizon in the laser science. The engineered materials of micro and/or microchip solid-state, ceramic and single-crystal, lasers can provide excellent spatial mode quality and narrow linewidths with enough power. High-brightness nature of these lasers has allowed efficient wavelength extension by nonlinear frequency conversion, from soft X-ray 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.



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.

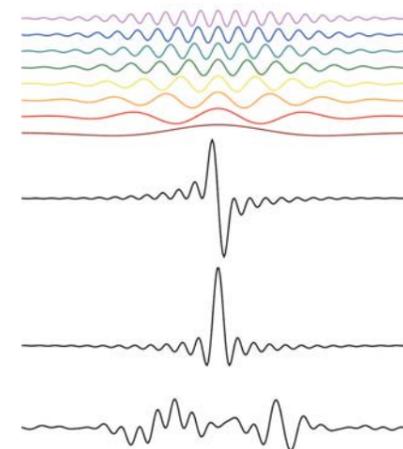


Advanced Laser Development

Ultrafast laser science

FUJI, Takao (Associate Professor)

mail:fuji@ims.ac.jp



Superimposition of light fields of various wavelengths (colored lines) with precisely controlled phases results arbitrary waveform synthesis (black lines).

Speed of ultrafast energy transfer from light to molecules (i.e. primary processes of photosynthesis, photoisomerization in visual pigments, etc.) is on the order of femtosecond (10^{-15} s). In our laboratory, we develop cutting edge lasers for such ultrafast molecular science, namely, femtosecond or attosecond (10^{-18} s) ultrashort pulse lasers. For example, arbitrary waveform synthesis can be performed with simultaneous generation of femtosecond light pulses in various wavelength regions and superimposition of them with precisely controlled phases. We would like to develop such advanced light control technology, which can push forward the research on ultrafast photochemical reactions.



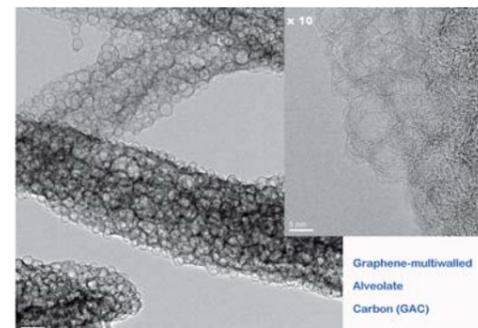
Extensive development of new molecules, molecular systems and their higher-order assemblies is being conducted. Their electric, photonic and magnetic properties, reactivities, and catalytic activities are being examined in an attempt to discover new phenomena and useful functionalities.

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



Metal acetylides composed of C₂ anions and metal cations produce various nanostructures characteristic of metal atoms. We have succeeded to synthesize "Graphene-walled Mesoporous Carbon Nano-Dendrite(MCND) with BET surface areas of 1600-2000 m²/g and Graphene-multiwalled Alveolate Carbon(GAC) with spherical cavities stacked together just like a honey-comb structure. As shown in the TEM images in the figure, GACs are composed of more than triple graphene walls. The outer-most sheets act as electron or hole transfer terminals to the contacting metal layers when we put metals in the cavities. These cavities possess holes for transferring ions from inside to outside through the solvents or electrolytes. The inner graphene sheet(s) acts as electric conductance layer. Since GAC is a three dimensional monolith with a size of 10-100μm, electric conductivity of GAC is good enough to be used as an ideal electrode material. In the cavities, one can store the metals or ions for batteries. The cavity also acts as catalytic terminals for hydrogen or oxygen fixation.

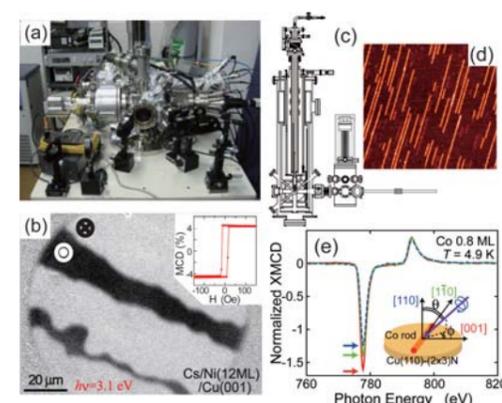


Electronic Structure

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



- Ultraviolet magnetic circular dichroism photoelectron emission microscope (UV MCD PEEM).
- First UV MCD PEEM image. The sample is 12 monolayer Ni on Cu(001) and shows upward and downward magnetic domains clearly.
- X-ray magnetic circular dichroism (XMCD) system with a superconducting magnet and a liq. He cryostat.
- STM image of Co nano-rods grown on Cu(001)-(2x3)N.
- 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.



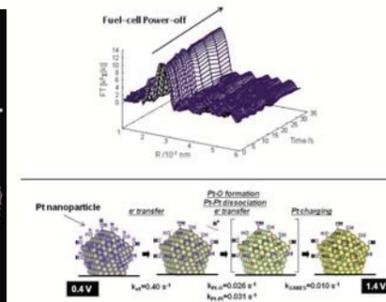
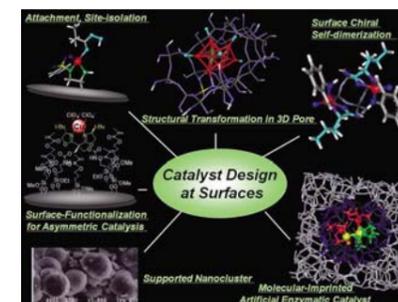
Electronic Structure

Surface-Mediated Catalyst Design for Highly Active and Selective Catalysis

TADA, Mizuki (Associate Professor)

mail:mtada@ims.ac.jp

Most of useful chemical products have been produced in the presence of heterogeneous catalysts and the design of novel catalysts for efficient catalysis is the state-of-art subject in chemistry. We have designed and prepared novel metal-complex catalysts on oxide surfaces by several unique techniques, surface molecular imprinting, surface chiral self-dimerization etc., and succeeded in preparing novel supported metal catalysts for direct phenol synthesis from benzene/O₂, CH₄ steam-reforming etc. In-situ characterization of active heterogeneous catalysts has been developed by XRD, solid-state NMR, FT-IR, Raman spectroscopy, ESR, and time-resolved XAFS.



1): Novel Catalyst Design at Solid Surface.

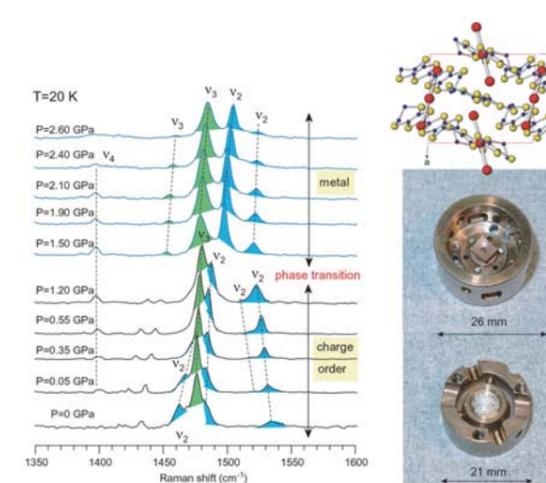
2): Deactivation Mechanism of Active Fuel-Cell Catalyst by In-situ Time-Resolved XAFS.

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 20K. 1 GPa corresponds to 104bar. This compound changes into metallic state above 1.5GPa. 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 and ferroelectric phase accompanying charge order.



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-known 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 attention by their possible functionality because of various electronic phases. Magnetic resonance is an advanced technique which enables us to clarify the character of materials by nuclear and/or electron magnets as probes without contact and destruction.



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

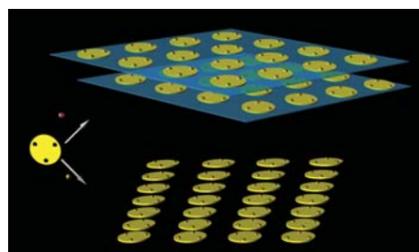
Molecular Functions

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 π -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.

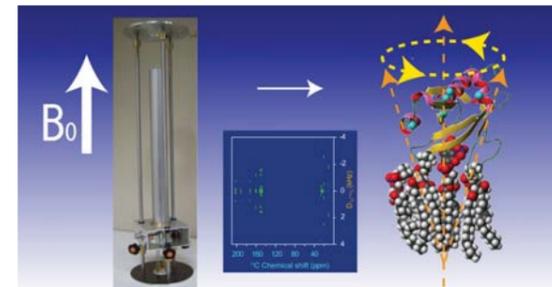
Molecular Functions

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.

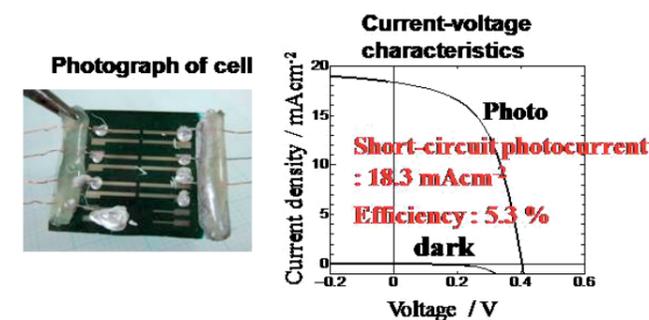
Molecular Nanoscience

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.

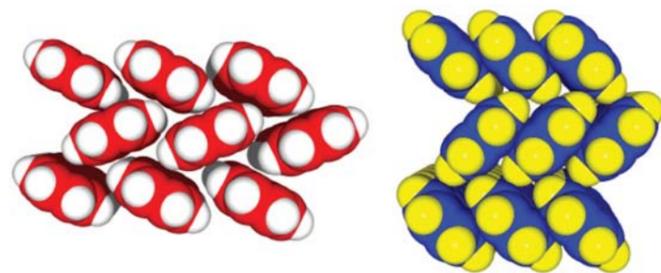
Molecular Nanoscience

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.



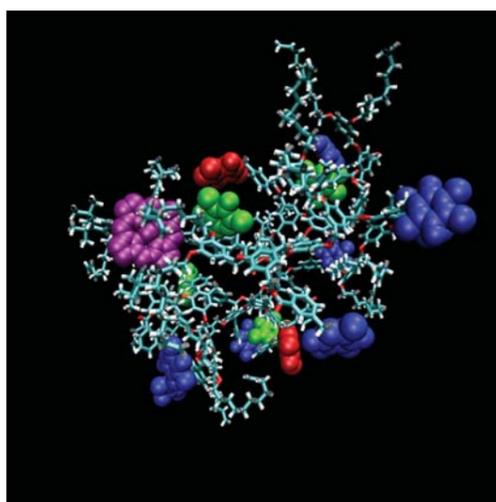
Crystal structures of pentacene and perfluoropentacene as the organic semiconductors.

Molecular Nanoscience

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.

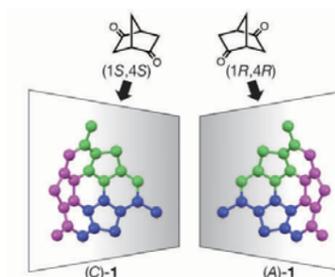


Molecular Nanoscience

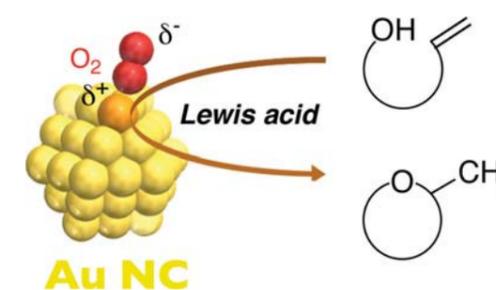
Science of Buckybowls and Development of Metal Nanocluster Catalyst

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

Bowl-shaped π -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.

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

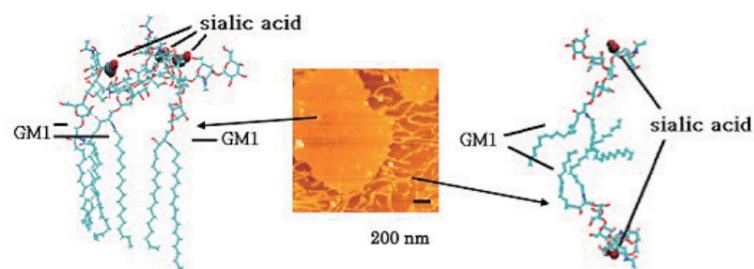
Developments of Neural Network Analyzer and Medical Molecular Science

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.



Aggregation of amyloid β ($A\beta$) is considered to be a hallmark of Alzheimer's disease. We have formed the GM1/SM/Chol planer lipid bilayer on the mica surface and found that unique phase separation occurs. If $A\beta$ is added on this surface, fibrillar $A\beta$ agglomerates forms selectively outside the triangular regions. This is due to the difference of the GM1 molecular conformations between inside and outside the triangular regions.

Biomolecular Sensing

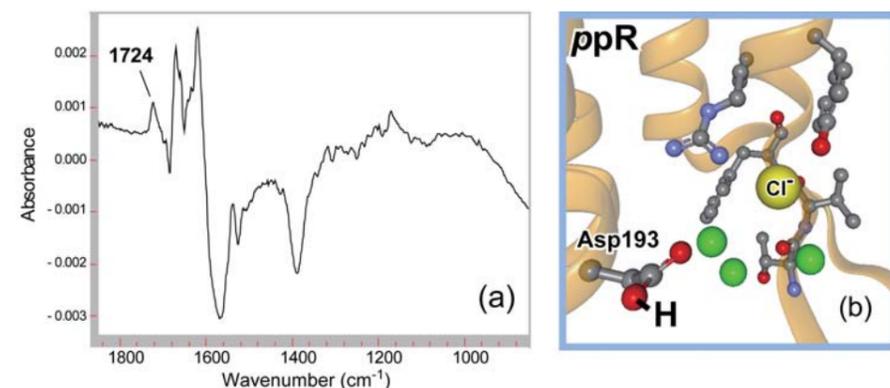
Investigation of Molecular Mechanisms of Transporters and Receptors in Cell Membrane

FURUTANI, Yuji (Associate Professor)

mail:furutani@ims.ac.jp



The cell, the elementary unit of the life, uptakes the nutrient and exhausts waste and its ion balance between the inside and outside is adjusted strictly. These are performed by membrane proteins such as channels and transporters. Moreover, cell sensor proteins detect various environmental changes. Our main goal is to clarify molecular mechanisms of transporters and receptors in cell membrane mainly by using infrared spectroscopy which is sensitive to the changes of molecular structures and environments.



(a) Chloride-ion binding induced difference infrared spectra of a membrane protein (*pharaonis* phoborhodopsin; light sensor in an archaeobacterium). The 1724-cm⁻¹ band was assigned to the protonated carboxylate group of Asp193.

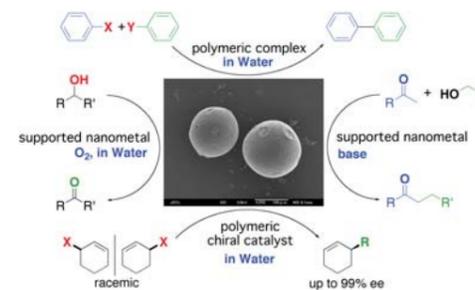
(b) The existence of hydrogen at Asp193, which has not been detected by X-ray crystallography, was revealed by infrared spectroscopy.

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.



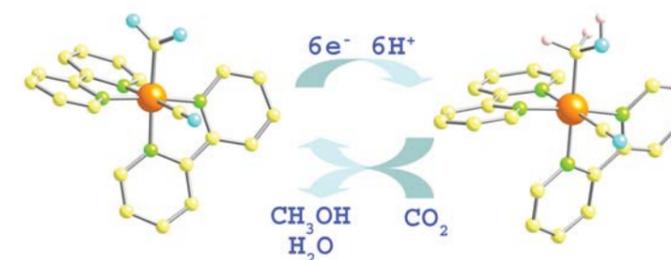
Functional Coordination Chemistry

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 issue that scientists now confront. We have been developing transition-metal complex catalysts for electro- and photochemical multi-electron reduction of CO₂ (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 CO₂ 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 CO₂ and electrochemical oxidation of organic compounds, respectively.



Multi-electron reduction of CO₂.

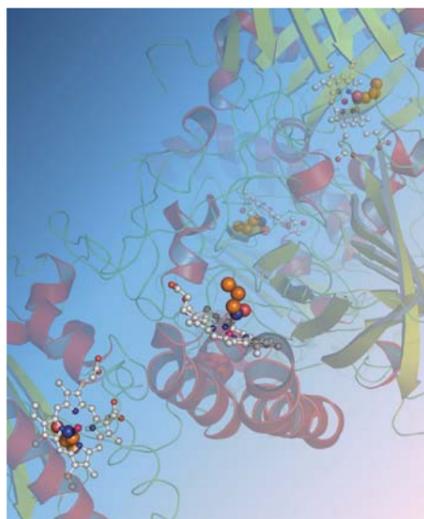


Biomolecular Functions

The Regulation of Biological Function by Metalloproteins

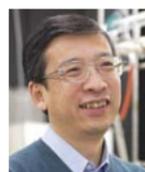
AONO, Shigetoshi (Professor)

mail:aono@ims.ac.jp http://groups.ims.ac.jp/organization/aono_g/



Structure of a novel heme enzyme, aldoxime dehydratase (OxdRE).

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.

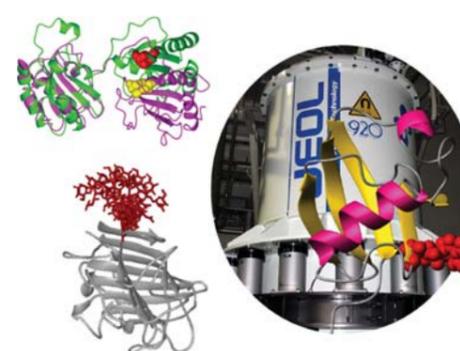


Biomolecular Functions

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

KATO, Koichi (Professor)

mail:kkatonmr@ims.ac.jp http://groups.ims.ac.jp/organization/kkato_g/



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.

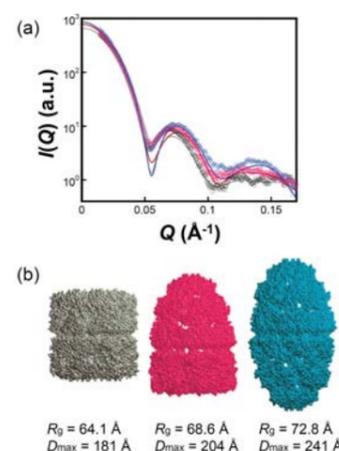


Biomolecular Functions

Molecular 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 (magenta), 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.



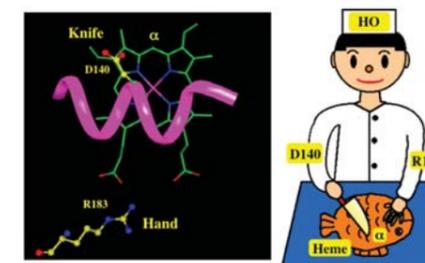
Biomolecular Functions

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 mechanism of heme oxygenase.

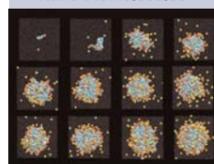
— Grand Challenge in Nanoscience —

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 devices, and so forth, by making the best use of the next generation supercomputer.

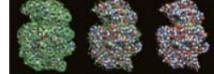
Next Generation Nano Information Function and Materials

Next Generation Nano Biomolecules

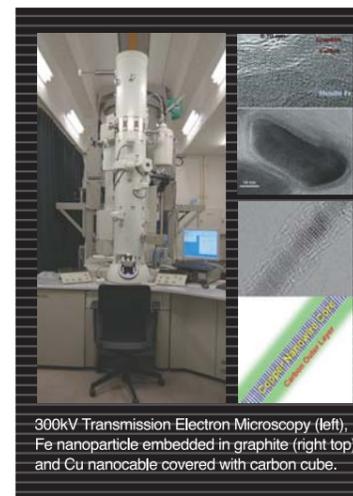
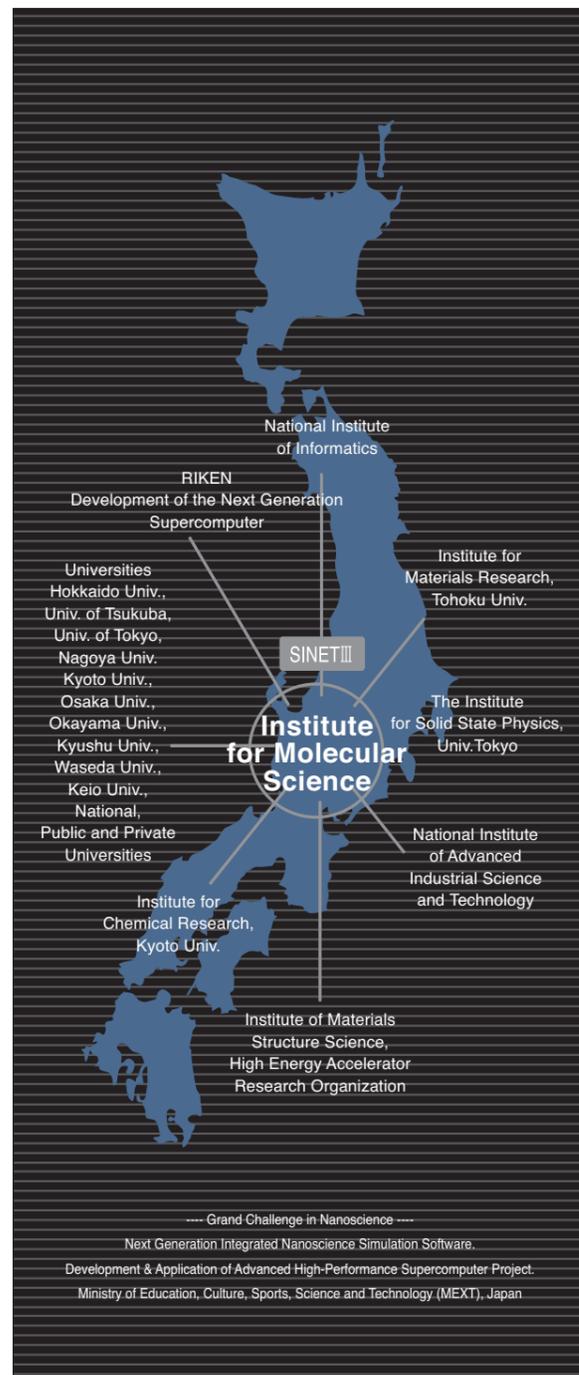


Drag Delivery System (Molecular Dynamics of Micelles)

Next Generation Energy



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



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 Common Utilization of Research Equipments

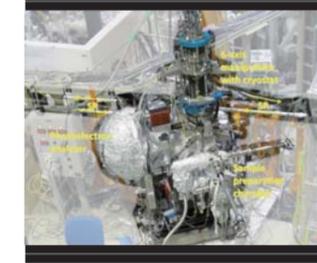
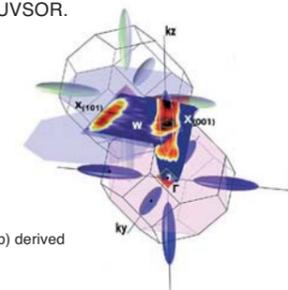
Academic and industrial activities in Chemistry in Japan have been highly influential over the past 30 years. Needless to say, it is highly important to improve the supporting environment for research and education in science and engineering. In particular, research equipments are advancing all the time 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. Since April 1st 2010, the project name has been changed as Inter-University Network for Common Utilization of Research Equipments and Promotion of Joint Research. 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

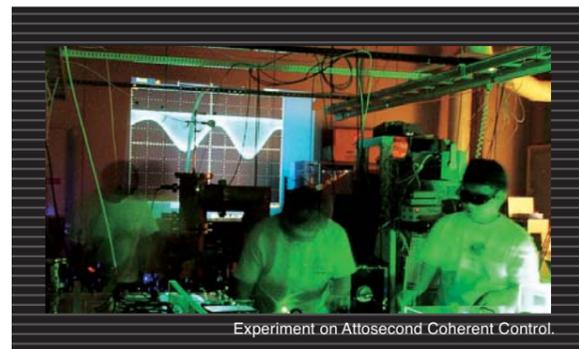
UVSOR Facility

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 electronic structure that is the origin of the functionalities of solids is directly observed by using SR. Our SR facility is called UVSOR.



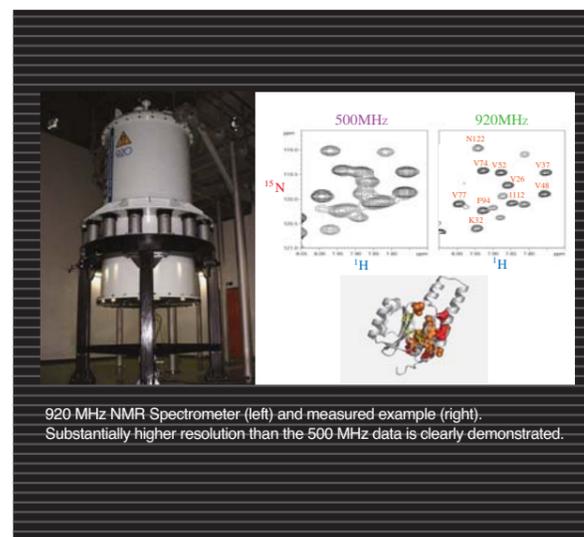
Extreme Photonics

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.



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 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.



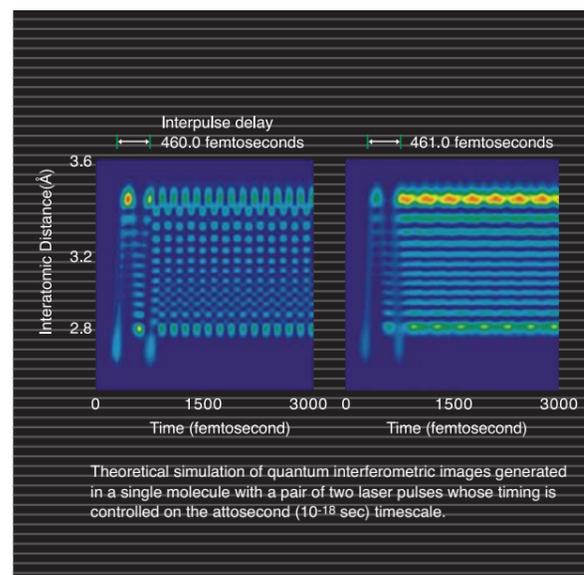
Laser Research Center for Molecular Science

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.

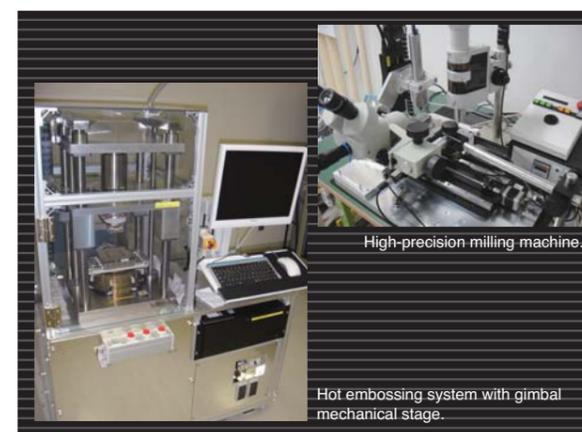
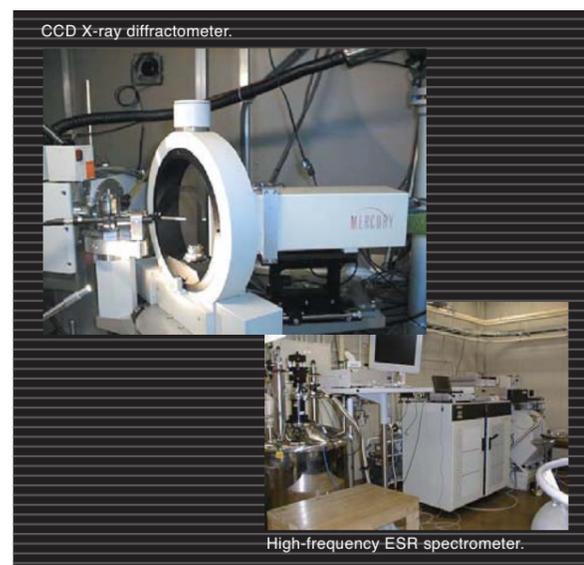


Microchip laser developed at the center.



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 circular dichroic spectrometer in Yamate campus and ESR, SQUID magnetometer, powder and single-crystal diffractometer, variable wave length picosecond laser system, fluorescence spectrophotometer, UV-VIS-NIR spectrophotometer, in Myodaiji campus. We mainly support a general-use experiment, and we often support a special one such as the experiment combining lasers and general-purpose machines. We provide liquid nitrogen and liquid helium using helium liquefiers. We also support the network sharing system of the chemistry-oriented instruments, which starts in the April of 2007.



Equipment Development Center

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

Okazaki Research Facilities

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 "High Performance Molecular Simulator" and "Super-High-Performance Molecular Simulator." Totally, they have performance as high as near 20 TFLOPS.



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

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).

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 countries. 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).

Korea	35	Nepal	2
USA	33	Vietnam	2
China	27	Poland	2
Germany	19	Russia	2
France	14	Ukraine	1
UK	11	Australia	1
Canada	10	Georgia	1
India	9	Singapore	1
Thailand	7	Pakistan	1
Taiwan	6	Bangladesh	1
Italy	4	Philippines	1
Indonesia	2	Finland	1
Holland	2	Bulgaria	1
Switzerland	2	Romania	1
Sweden	2		
Total 201			

Highly capable personnel nurtured by abundant research resources

Personnel Training : Education in Graduate School

IMS promotes pioneering and outstanding researches by young scientists as a core academic organization in Japan. IMS trains graduate students in 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, Colloquia and Molecular Science Forum to which speakers are invited from within Japan and all over the world, as well as other conferences held in IMS, graduate students have regular opportunities to be exposed to valuable information related to their own fields of researches 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 at facilitating their potential to deliver outstanding scientific contributions.

For more details on Departments of Structural Molecular Science and Functional Molecular Science, young scientists are encouraged to visit IMS through many opportunities such as 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 intentions of cultivating new integrative research fields and promoting academic excellence through its doctoral course programs that are also open to foreign students.

The university is based in Hayama, 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 fields of studies.

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, 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 200, 120, 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.

Now, Myodaiji lodge is under construction to build the new dormitory for long stay. It'll be available from August 2010.



■ Councillors

Anthony John Stace Professor, University of Nottingham
Jean-Pierre Sauvage Professor, University Louis Pasteur (Strasbourg I)

■ Advisory Committee

EBATA, Takayuki Professor, Graduate School of Science, Hiroshima University
FUKE, Kiyokazu Professor, Graduate School of Science, Kobe University (Vice chair)
MORI, Takehiko Professor, Graduate School of Science and Engineering, Tokyo Institute of Technology
SHINOHARA, Hisanori Professor, Department of Chemistry / Institute for Advanced Research, Nagoya University
TSUKUDA, Tatsuya Professor, Catalysis Research Center, Hokkaido University
UEMURA, Daisuke Professor, Faculty of Science and Technology, Keio University
WATANABE, Yoshihito Professor, Vice-President, Nagoya University
YAMAGATA, Yuriko Professor, Faculty of Medical and Pharmaceutical Science, Kumamoto University
YAMANOUCI, Kaoru Professor, Graduate School of Science, Tokyo University
YAMASHITA, Masahiro Professor, Graduate School of Science, Tohoku University
AONO, Shigetoshi Professor, Okazaki Institute for Integrative Bioscience
HIRATA, Fumio Professor, Institute for Molecular Science
KOSUGI, Nobuhiro Professor, Institute for Molecular Science (Chair)
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
SAITO, Shinji Professor, Institute for Molecular Science
TANAKA, Koji Professor, Institute for Molecular Science
UOZUMI, Yasuhiro Professor, Institute for Molecular Science
YOKOYAMA, Toshihiko Professor, Institute for Molecular Science

Personnel and Budget

Staff (as of April, 2010)		Grants-in-Aid (2009)*	
			(Thousand yen)
Director-General	1	Grant-in-Aid Scientific Research (KAKENHI, MEXT and JSPS)**	349,661
Professors	15 (10)	Joint Research	33,292
Associate Professors	16 (6)	CREST, PRESTO, others(JST)***	158,031
Assistant Professors	42	Special Coordination Funds for Promoting Science and Technology from MEXT***	434,765
Technical Professors	38 (1)	Others***	93,757
Total	112 (17)	Total	1,069,506

Budget (2009)		(Thousand yen)	
Personnel	1,207,802		
Research	2,090,047		
Facility	607,060		
Total	3,904,909		

() Indicates the number of adjunct professors excluded.

* Included in the left table
** Including indirect expenses
*** Including contract-based research and indirect expenses
MEXT : Ministry of Education, Culture, Sports, Science and Technology
JSPS : Japan Society for the Promotion of Science
JST : Japan Science and Technology Agency

