

## 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 conduction 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.

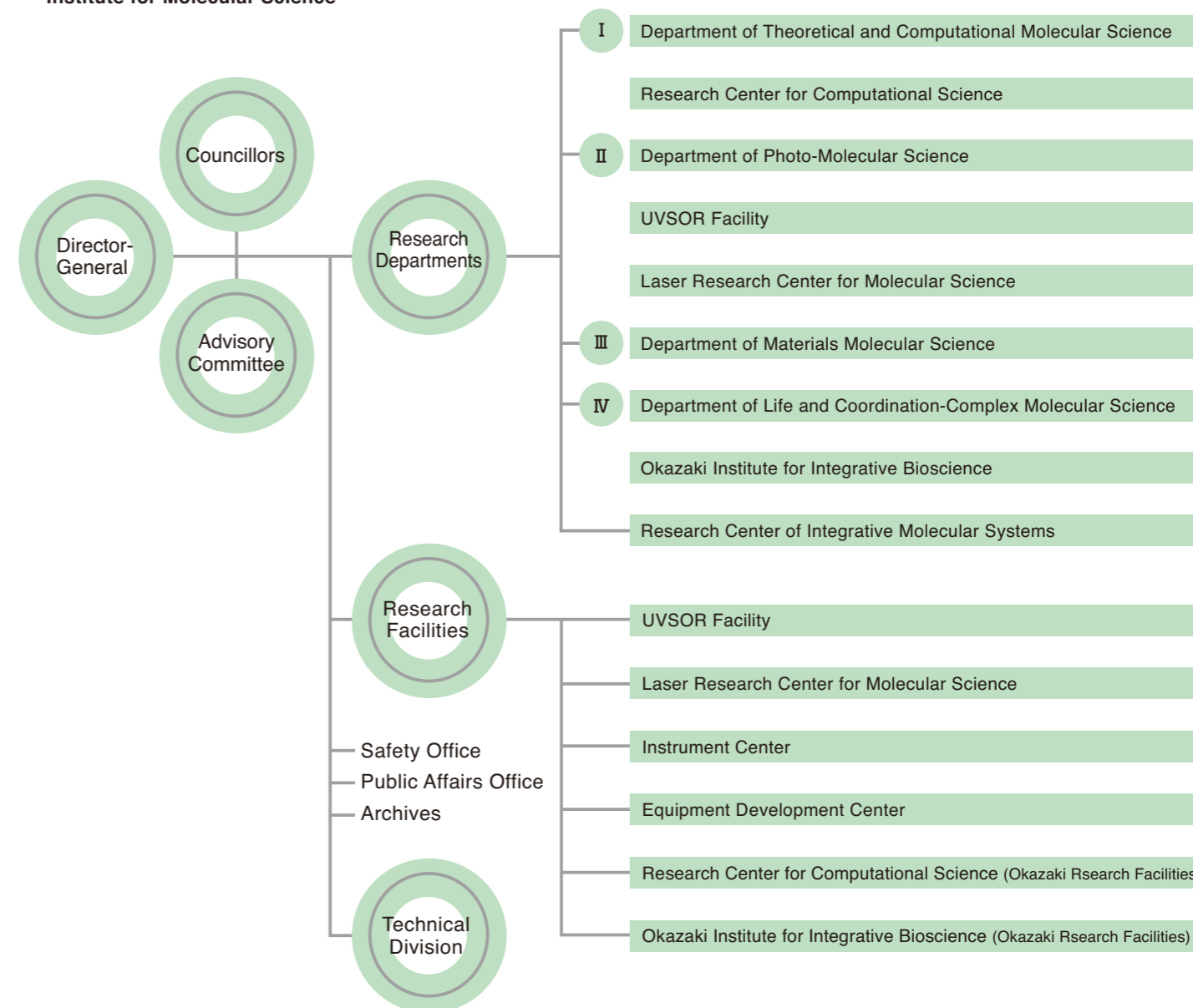
To facilitate the new field of molecular science, the IMS just launched a new research center, “Research Center for Integrative Molecular Systems (CIMoS),” on April 2013 (<http://cimos.ims.ac.jp>). The mission of CIMoS is to analyze molecular systems in nature to learn the “wisdom of molecules” for sharing and controlling the information between different spatiotemporal hierarchies, with the ultimate goal of creating flexibly but robustly functionalized molecular systems on the basis of these findings. The CIMoS will be the core center in IMS, to which almost half of all its faculties will precipitate. The CIMoS and the rest of the IMS faculties, who are expanding potentialities of molecules by reaching to the limits in precision of measurements and by achieving ultimate control over molecular systems, will go for a new “investigative adventure” on molecular science, for the future benefit of all people.

April, 2013

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 and Research Facilities. Technical groups primarily belong to one of the joint research facilities and also take care of 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 two 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(-March 2013)  
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  
Apr. 2013 Research Center of Integrative Molecular Systems established

## Describing invisible and intricate molecules

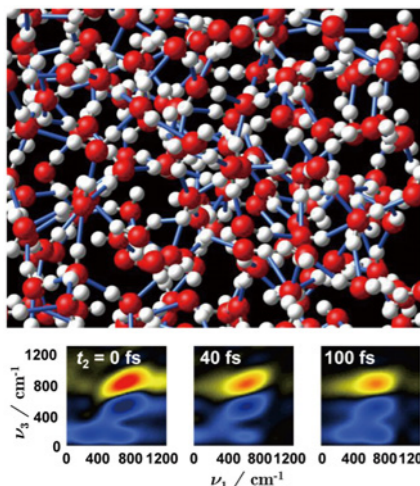
It is our ultimate goal to develop theoretical and computational methodologies that include quantum mechanics, statistical mechanics, and molecular simulations in order to understand the structures and functions of molecules in gasses and condensed phases, as well as in bio and nano systems.

### Theoretical Molecular Science I

#### Theoretical Studies on Temporal and Spatial Heterogeneous Dynamics

SAITO, Shinji ( Professor )

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A snapshot of liquid water (upper) and time-dependence of two-dimensional IR spectra 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 furthermore, produce various properties and functions. Knowledge of temporal and spatial heterogeneous dynamics is essential to understand the dynamics and chemical reactions in these systems. We have been investigating fluctuations and chemical reactions in the condensed phases by using molecular dynamics simulations and electronic calculations. In addition, fluctuations and energy relaxations have been examined in terms of theoretical nonlinear spectroscopies.



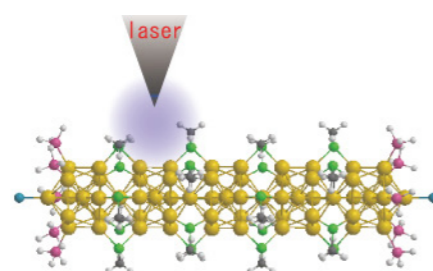
### Theoretical Molecular Science I

#### Theory of Photoinduced Quantum Dynamics in Nanostructures

NOBUSADA, Katsuyuki ( Associate Professor )

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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.

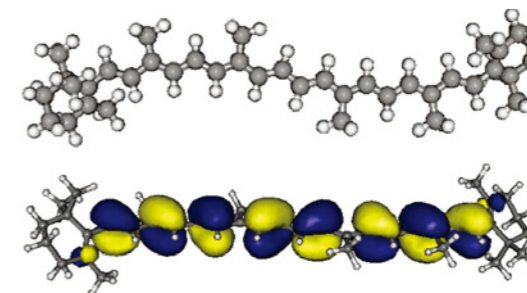
### Theoretical Molecular Science I

#### Advanced Electronic Structure Theory for Predictive Quantum Chemistry

YANAI, Takeshi ( Associate Professor )

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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.



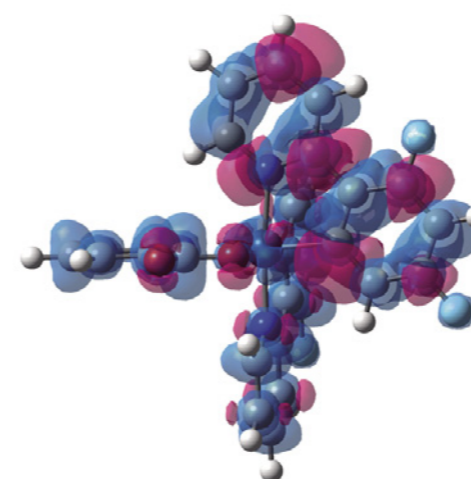
Molecular structure and molecular orbital of beta carotene.

### Computational Molecular Science

#### Exploring New Field of Theoretical Chemistry Based on Electronic Structure Theory

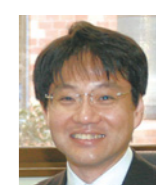
EHARA, Masahiro ( Professor )

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.

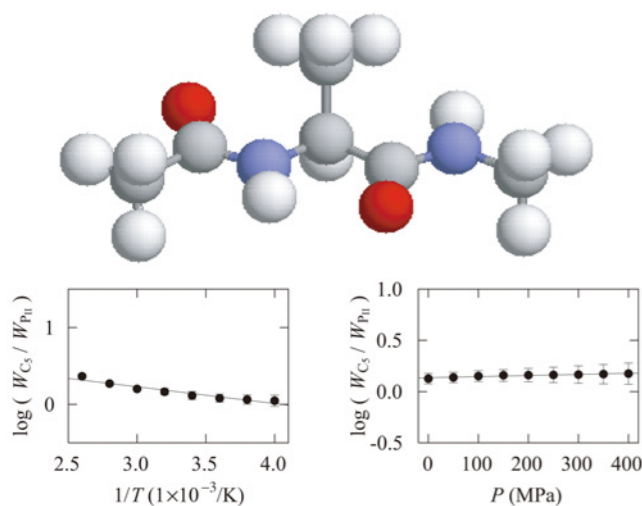


## Computational Molecular Science

### Simulations of Biomolecules under Extreme Conditions

OKUMURA, Hisashi ( Associate Professor )

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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.

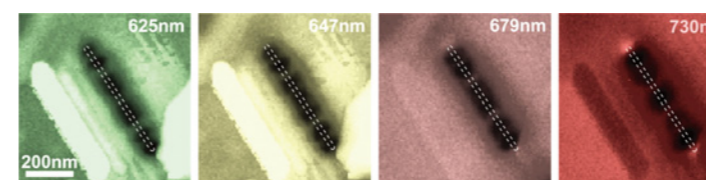
## Photo-Molecular Science I

### Exploring Nanomaterials by Novel Optical Microscopes

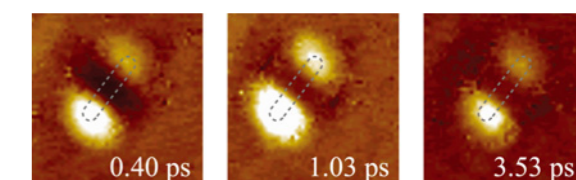
OKAMOTO, Hiromi ( Professor )

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 of observation.



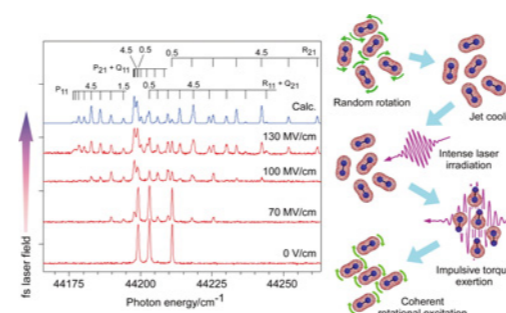
Images of ultrafast dynamic behavior of a nanometer-sized (length 300nm) metal rod. 1ps = 1000fs = 1/1,000,000,000,000s.

## Photo-Molecular Science I

### Design and Reconstruction of Molecular Quantum States of Motion

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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.



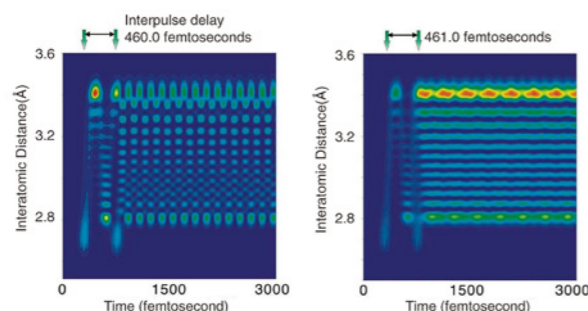
## Photo-Molecular Science II

### Attosecond Quantum Engineering

**OHMORI, Kenji ( Professor )**

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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.



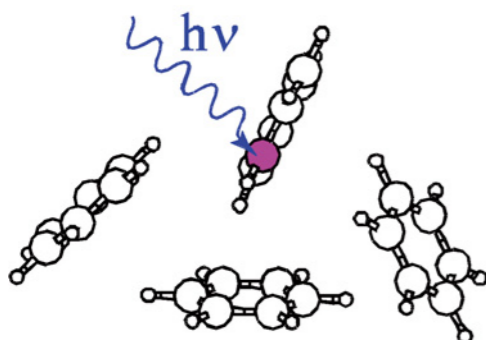
Theoretical simulation of quantum interferometric images generated in a single molecule with a pair of two laser pulses whose timing is controlled on the attosecond ( $10^{-18}$  sec) timescale.

## Photo-Molecular Science III

### Molecular Inner-Shell Spectroscopy

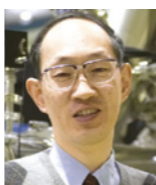
**KOSUGI, Nobuhiro ( Professor )**

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Site-selective inner-shell excitations in molecular clusters.

Inner-shell spectroscopy is applied to the molecular system, such as molecular clusters, solutions, and 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. 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 (X-ray absorption, X-ray emission, and photo electron) to reveal local electronic structures determining various kinds of interesting molecular properties.



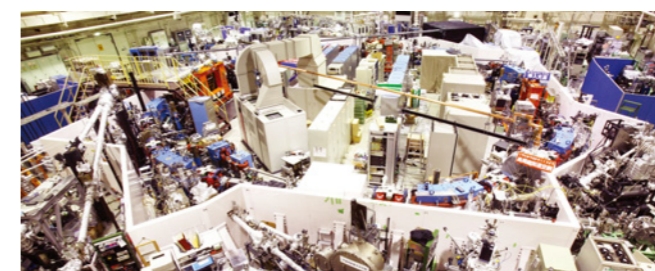
## Advanced Accelerator Research

### Light Source Developments by Using Relativistic Electron Beam

**KATOH, Masahiro ( Professor )**

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UVSOR is a synchrotron light source to provide low energy synchrotron light from terahertz range to soft X-ray range. Although it was constructed about 30 years ago, its performance is still in the world top level. This is a result of the continuous effort on improving the machine. Our research group is developing accelerator technologies toward producing bright and stable synchrotron light, such as high brightness electron beam optics, novel insertion devices or state-of-the-art beam injection technique. We are also developing novel light source technologies toward producing synchrotron radiation with various properties such as free electron laser, coherent synchrotron radiation and laser Compton gamma-rays. We are also investigating future light sources for the facility, such as ultra-high brilliance light source or a free electron laser on a linear accelerator.



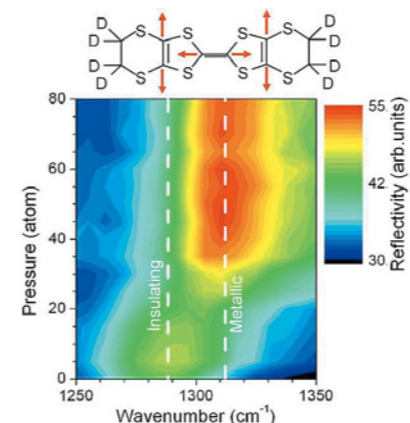
UVSOR-II Electron Storage Ring.

## Advanced Solid State Physics

### Development of Functionality of Solids 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.

Functionalities of solids and thin films, such as conductivity and magnetism, originate from the electronic structure near the chemical potential as well as the Fermi level. We explore the origins of the functionalities and develop new physical properties from the electronic structure observed by using angle-resolved photoemission spectroscopy (ARPES) and optical conductivity measurements. We also develop new experimental techniques of three-dimensional ARPES, and optical measurements at extreme conditions, such as high pressure, high magnetic field and very low temperature using high-brilliant synchrotron radiation. Such new methodology certainly gives us precise and/or hidden information of electronic structure that cannot be observed by existing techniques.

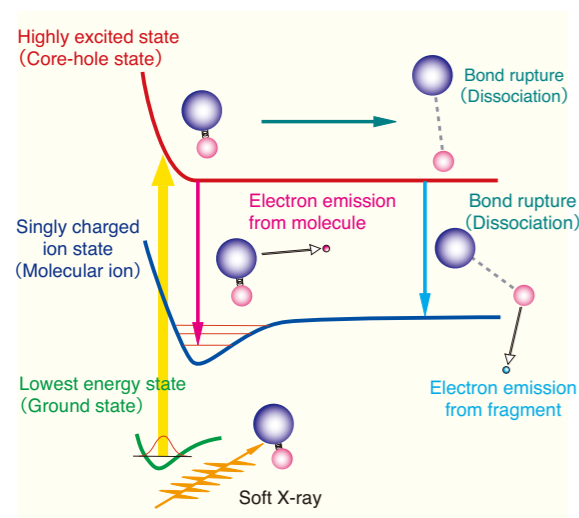


## Advanced Photochemistry

### Dynamical Processes Arising from Inner-Shell Hole Creation in Molecules

SHIGEMASA, Eiji ( Associate Professor )

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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.



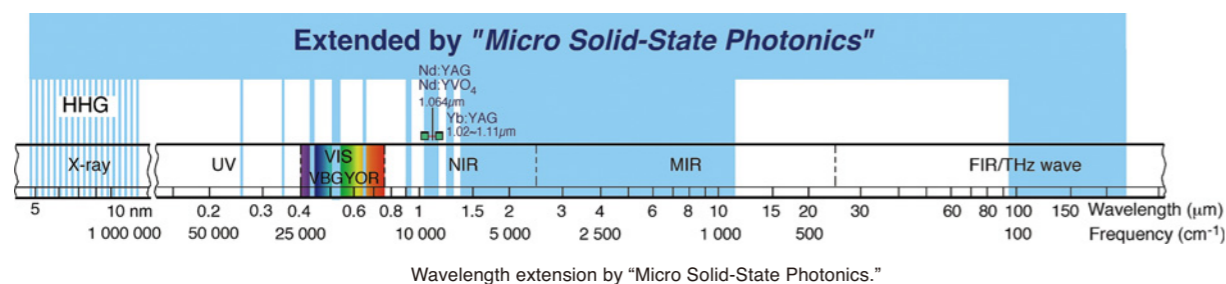
## Advanced Laser Development

### Micro Solid-State Photonics

TAIRA, Takunori ( Associate Professor )

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"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.



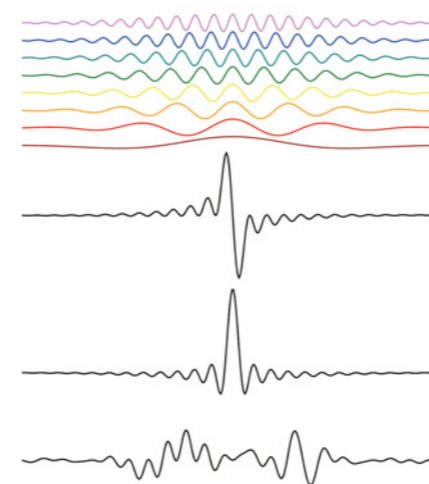
Wavelength extension by "Micro Solid-State Photonics."

## Advanced Laser Development

### Ultrafast laser science

FUJI, Takao ( Associate Professor )

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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 (e.g. 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.



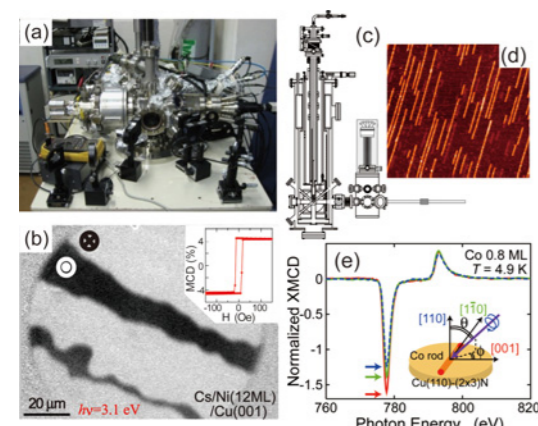
Extensive development of new molecules, molecular systems and their higher-order assemblies is being conducted. Their electric, photonic and magnetic properties, reactivities, and catalytic activities are being examined in an attempt to discover new phenomena and useful functionalities.

### Electronic Structure

#### Characterization of Magnetic Thin Films Using Photons

**YOKOYAMA, Toshihiko ( Professor )**

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- (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

#### Electronic Properties Investigation of Molecular Conductors by Magnetic Resonance

**NAKAMURA, Toshikazu ( Associate Professor )**

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

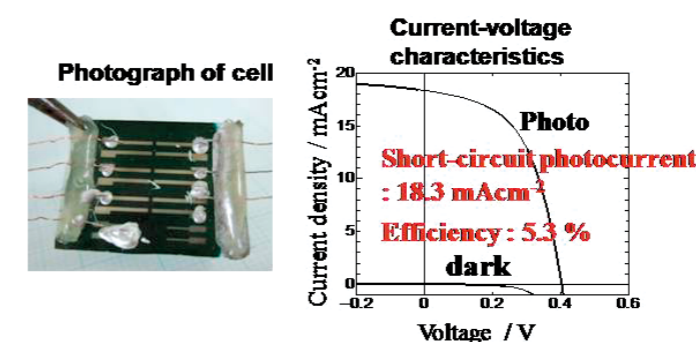
### Molecular Functions

#### Organic Electronic Devices

**HIRAMOTO, Masahiro ( Professor )**

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Organic EL television has been commercialized. 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, pn-control nanostructure design.



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

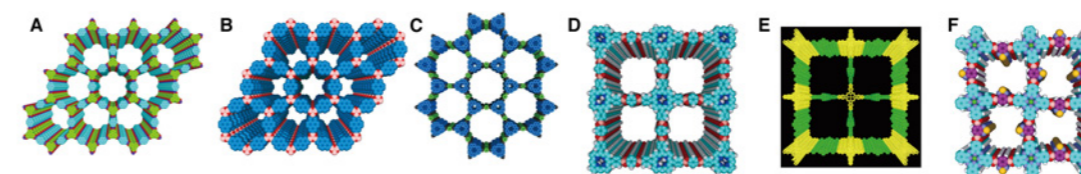
### Molecular Functions

#### Two-Dimensional Polymers and Porous Organic Frameworks

**JIANG, Donglin ( Associate Professor )**

mail:jiang@ims.ac.jp [http://groups.ims.ac.jp/organization/jiang\\_g/Lab.html](http://groups.ims.ac.jp/organization/jiang_g/Lab.html)

Our laboratory focuses on the design, synthesis, and functional exploration of novel porous organic architectures, including two-dimensional polymers, covalent organic frameworks, and conjugated microporous polymers. Two-dimensional polymers allow the integration of organic units into periodically ordered structure with the intra-sheet periodicity extended to a third dimension upon stack, thus forming unique  $\pi$  columnar arrays and one-dimensional nanochannels. Conjugated microporous polymers combine inherent microporosity with extended  $\pi$  conjugation, offering a unique molecular space. We are exploring these porous organic polymers for gas storage, green catalysts, light harvesting, light emitter, photoinduced energy transfer, charge separation, photo-energy conversion, and electric energy storage.



Two-dimensional polymers feature periodically aligned  $\pi$  columnar arrays and ordered one-dimensional nanochannels

Two-Dimensional Polymers.

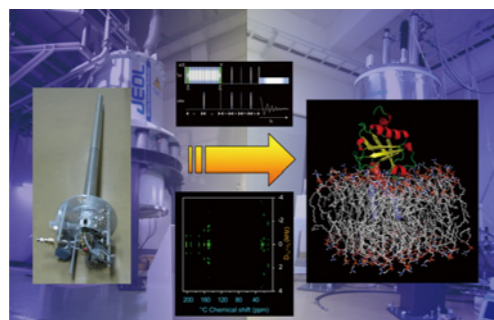
## Molecular Functions

### Methodology Developments of Solid State NMR for Biomolecules

**NISHIMURA, Katsuyuki ( Associate Professor )**

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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 probes.  
(Middle) Pulse sequence and 2D NMR spectrum.  
(Right) Peripheral membrane protein bound to lipid bilayers.

## 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.

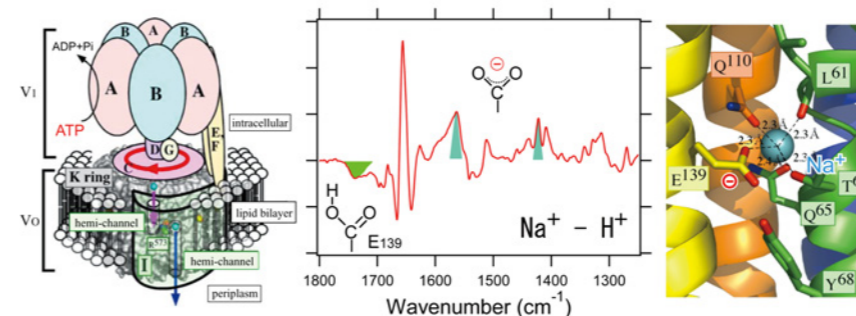
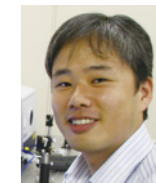
## Biomolecular Sensing

### Investigation of Molecular Mechanisms of Transporters and Receptors in Cell Membrane

**FURUTANI, Yuji ( Associate Professor )**

mail:furutani@ims.ac.jp

Membrane proteins are important for homeostasis of living cells, which work as ion channel, ion pump, various types of chemical and biophysical sensors, and so on. These proteins are considered as one of important targets for biophysical studies. However, their molecular mechanisms have not been studied well, because X-ray crystallography and NMR spectroscopy are hard to access them in general. Our main goal is to clarify molecular mechanisms of transporters and receptors in cell membrane mainly by using stimulus-induced difference infrared spectroscopy which is sensitive to the structural and environmental changes of organic and bio-molecules.



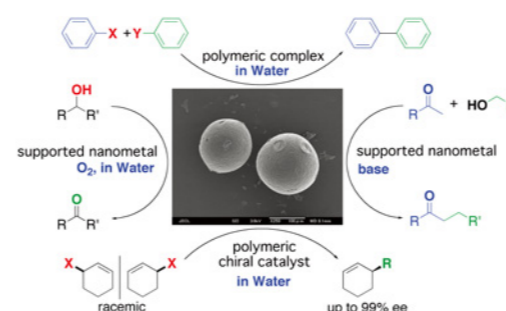
(left) Schematic structure of whole V-ATPase protein complex (center) Sodium ion binding induced difference infrared spectrum (Y. Furutani et al., *J. Am. Chem. Soc.* 2011). The green and cyan colored bands are assigned to protonated and deprotonated carboxylic acid residues of Glu139 in K-ring, respectively. (right) Sodium ion binding site revealed by X-ray crystallography on K-ring.

## 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/](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);  $\alpha$ -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.





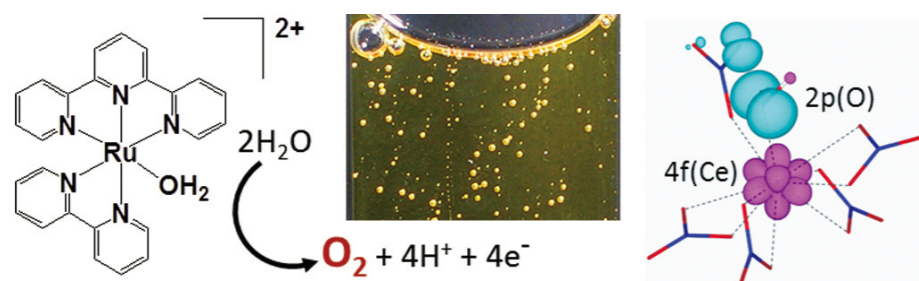
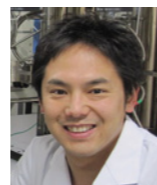
## Functional Coordination Chemistry

### Development of Functional Metal Complexes for Artificial Photosynthesis

MASAOKA, Shigeyuki ( Associate Professor )

mail:masaoka@ims.ac.jp

Visible-light-induced water splitting reaction has attracted much attention due to its potential application toward artificial solar energy conversion and storage. This water-to-fuels conversion consists of the two half-cell reactions, reduction of water to H<sub>2</sub> and subsequent oxidation to O<sub>2</sub>. We have reported that some mononuclear ruthenium complexes with an aqua ligand exhibit surprisingly high catalytic activity towards O<sub>2</sub> evolution from water in the presence of Ce<sup>4+</sup>. This finding became a significant breakthrough in this field because it has long been believed that the water oxidation is much more effectively catalyzed by dinuclear or tetranuclear metal complexes.



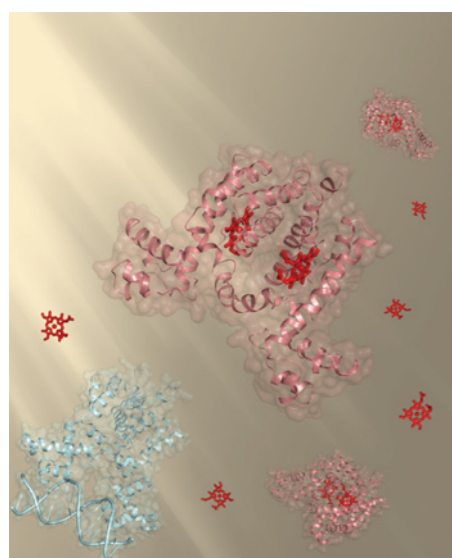
The mononuclear ruthenium complex active for O<sub>2</sub> evolution (left), bubbles of oxygen gas evolved (middle), and the spin density distribution of [Ce(OH)(NO<sub>3</sub>)<sub>5</sub>]<sup>2-</sup> (right). The radical character provided by the hydrocerium(IV) ion plays an important role in the catalysis of the mononuclear ruthenium complexes.

## 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/



HrtR that regulates heme homeostasis in cells dissociates from DNA to induce the expression of the heme transporter system upon sensing heme molecules.

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.

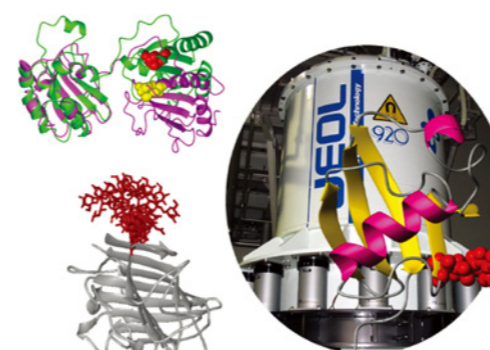


## Biomolecular Functions

### 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.



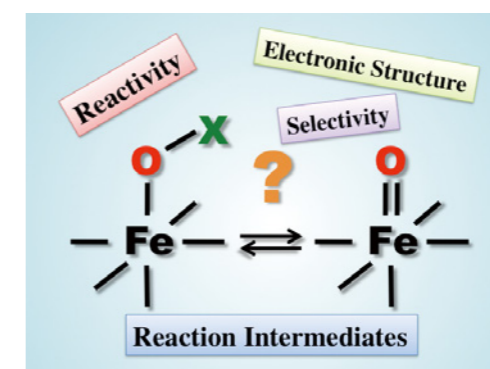
## Biomolecular Functions

### Molecular 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 controlling reactivity and selectivity.

The mission of CIMoS is to analyze molecular systems in nature to find the logic behind the sharing and control of information between the different spatiotemporal hierarchies, with the ultimate goal of creating novel molecular systems on the basis of these findings.

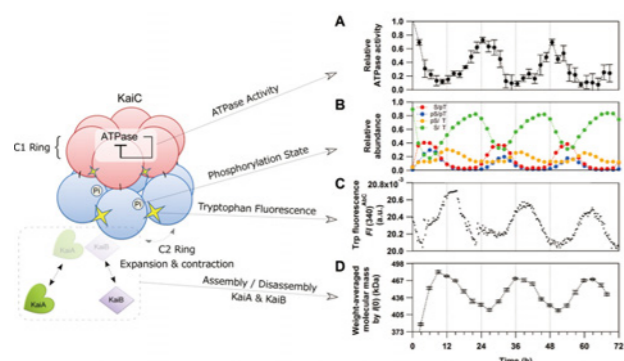
Division of Trans-Hierarchical Molecular Systems

### Molecular Origin of 24 h Period in Cyanobacterial Protein Clock

**AKIYAMA, Shuji ( Professor )**

mail:akiyamas@ims.ac.jp

KaiC, a core protein of the circadian clock in cyanobacteria, undergoes rhythmic structural changes over approximately 24 h in the presence of KaiA and KaiB (Kai oscillator). This slow dynamics spanning a wide range of both temporal and spatial scales is not well understood, and is central to a fundamental question: what determines the temperature-compensated 24 h period? The Kai oscillator reconstitutable in vitro is advantageous for studying its dynamic structure through a complementary usage of both X-ray crystallography and solution scattering, its transient response by using physicochemical techniques, and its molecular motion through a collaborative work with computational groups. We hope you will join us and enjoy the frontier in molecular science of circadian time-keeping system.



Circadian ticking of cyanobacterial clock protein KaiC (Y. Murayama et al. *EMBO J.*, **30**, 68-78 (2011)). The C1 and C2 domains in each protomer of KaiC are drawn as red and blue spheres, respectively. Expansion and contraction motions of the C2 ring (B, C) in solution serves as a timing cue for assembly/disassembly of KaiA and KaiB (D), and is interlocked with its C1 ATPase under a control of negative-feedback regulation (A).

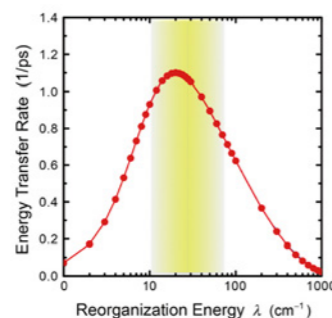
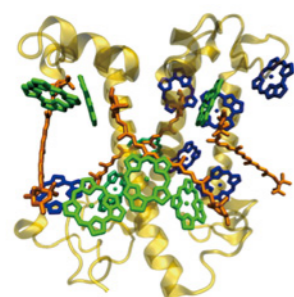
Division of Trans-Hierarchical Molecular Systems

### Unveiling Responsive and Autonomous Behaviors of Molecular Systems through Investigating Photosynthetic Light Harvesting

**ISHIZAKI, Akihito ( Research Associate Professor )**

mail:ishizaki@ims.ac.jp

Molecular systems function efficiently and robustly even with exposure to severely disturbing environmental noises. Further, they adapt and reprogram their functions in response to nonperturbative change of environments. Through investigating functionality of photosynthetic light harvesting systems with the help of condensed phase quantum dynamical theories and molecular simulations, we tackle unveiling design principles of such responsive and autonomous behaviors that molecular systems generally exhibit. Although our research would necessitate a variety of mathematical techniques and high-performance computing, our aim is to provide intuitive models to distill their intricate behaviors into a series of physicochemical concepts.



(LEFT) The crystal structure of a monomeric unit LHCII isolated from spinach. The relative position of the chlorophylls (chlorophylls in green & blue and carotenoids in orange) is drawn with the  $\alpha$ -helices spanning the thylakoid membrane. It is considered to vary its functions in response to nonperturbative change of environments, e.g. low light intensity v.s. high light intensity. (RIGHT) Rate of electronic excitation transfer between two pigments as a function of reorganization energy of their protein environment. The transfer rate is optimized in the parameter region corresponding to natural photosynthetic light harvesting systems (colored in yellow).

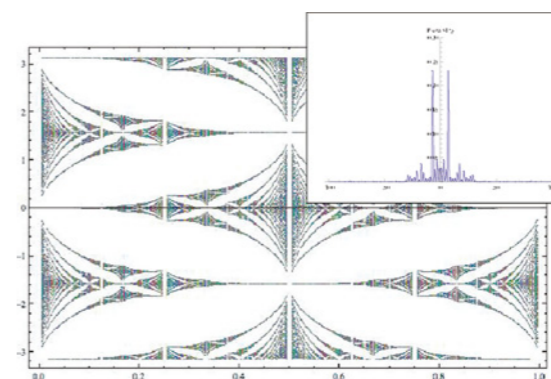
Division of Trans-Hierarchical Molecular Systems

### Construction of Ultimate Measurement for Molecule – Who has seen a molecule? –

**SHIKANO, Yutaka ( Research Associate Professor )**

mail:yshikano@ims.ac.jp

While everybody seem to believe the existence of the molecule, nobody have not directly seen the molecule itself. Furthermore, the fundamental law of the molecule is quantum mechanics. Its shape is rapidly changed. The aim of my study is to find the limitation/constraint of the measurement for the molecule. Throughout my study, I would like to ask what is understandable for the molecules in the research fashion of the huge data science and the highly performed numerical simulation.



Example of the complex but regular phenomena from the simple law: Hofstadter's butterfly and Multi-fractal structure.

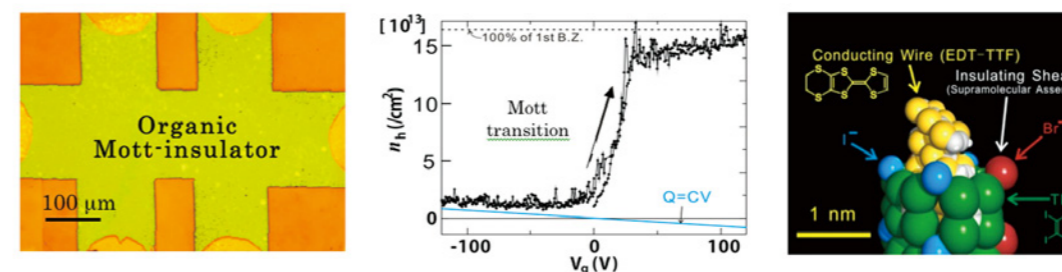
Division of Functional Molecular Systems

### Development of new $\pi$ -electronics using molecular conductors

**YAMAMOTO, Hiroshi ( Professor )**

mail:yhiroshi@ims.ac.jp

Our group is trying to establish new concepts of electronics based on  $\pi$ -electrons in soft materials such as organic molecules. Because of the low-dimensionality of  $\pi$ -electrons, the electric properties of these materials can be quite different from those of conventional Si devices. For example, the Coulomb interaction among electrons is enhanced to result in many unusual behaviors such as superconductivity. These phenomena can be controlled by using FET device structures and/or supramolecular architectures. Our research aims at paving the way to new nano-scale devices or quantum computers. (FET = Field effect transistor)



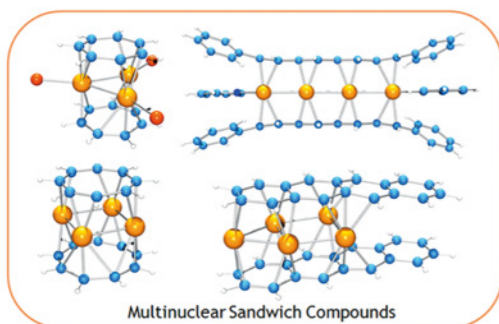
(left) Microscope image for Mott-FET device. (center) Change of the carrier density observed at the organic interface upon the Mott-transition. (right) CPK modeling for supramolecular nanowire. Yellow molecules constitute one-dimensional conducting wire while green molecules aggregate to form an insulating sheath.

Division of Functional Molecular Systems

## Synthetic Inorganic and Organometallic Chemistry, Catalysis, and Materials Science

MURAHASHI, Tetsuro ( Professor )

mail:mura@ims.ac.jp



Several examples of multinuclear sandwich complexes which our group isolated and structurally characterized.

Our research focuses on developing fundamental chemistry of transition metal complexes. We develop new synthetic methods realizing unprecedented transition metal complexes. Ongoing work in our laboratory concerns chemistry of extended multinuclear sandwich compounds. We recently revealed the existence of stable multinuclear sandwich complexes, despite a basic assumption that only one or two metal atoms can be incorporated between two parallel unsaturated hydrocarbon ligands in a sandwich compound. We also explore reactivity patterns and physical properties of novel transition metal compounds including discrete palladium clusters.



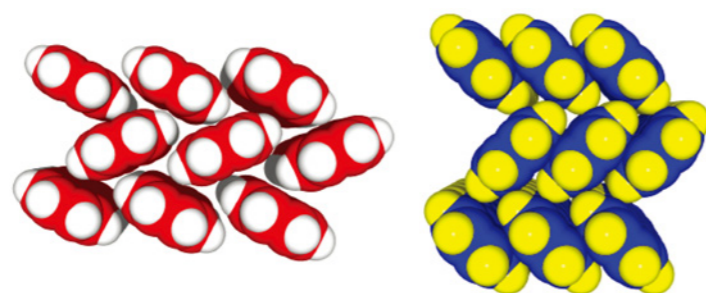
Division of Functional Molecular Systems

## 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.

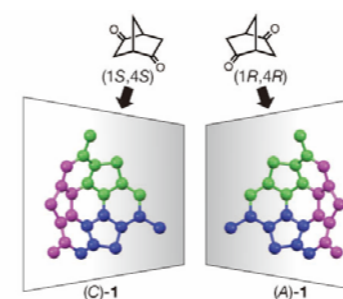
Division of Functional Molecular Systems

## Science of Buckybowls and Development of Metal Nanocluster Catalyst

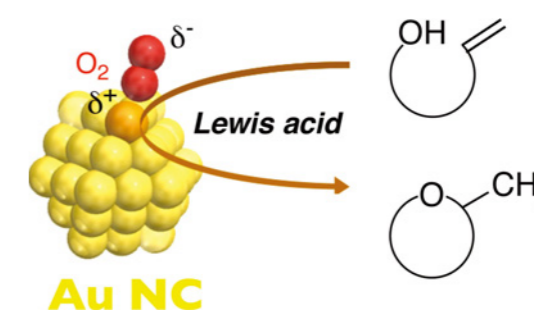
SAKURAI, Hidehiro ( Associate Professor )

mail:hsakurai@ims.ac.jp [http://groups.ims.ac.jp/organization/sakurai\\_g/english/](http://groups.ims.ac.jp/organization/sakurai_g/english/)

Bowl-shaped  $\pi$ -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.

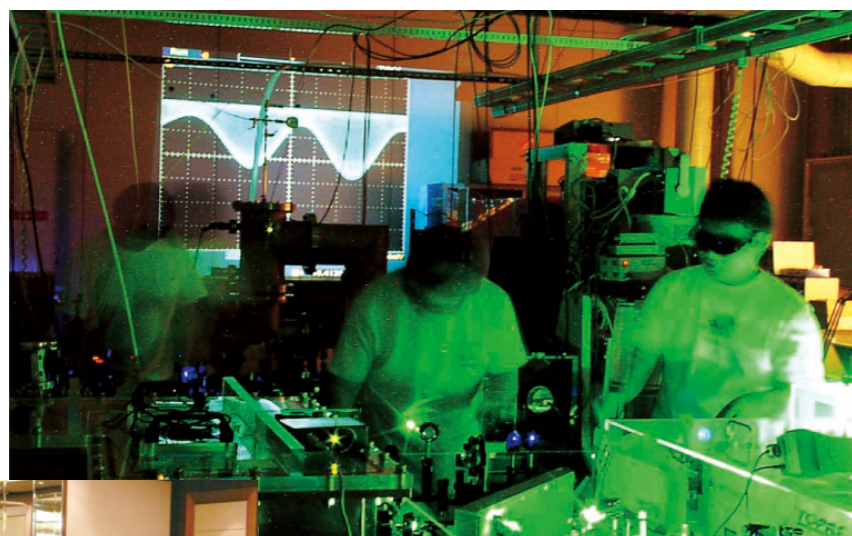
## Our Mission

It is our mission to enhance the progress of molecular science covering broader research areas, via mutual exchange of human resources among all the universities in this country and international cooperation with worldwide scientific society. For this purpose, IMS has been actively fostering many joint programs, with aiming to founding the research cores in advanced molecular science, providing maximum opportunities for collaborative researches and full utilization of IMS' state-of-the-art facilities to all the Japanese researchers in the field, and constructing a solid research network among the international scientific community.

### Founding the research cores in advanced molecular science

IMS has been conducting various joint research programs in collaboration with universities and other research institutes. In the field of photo-molecular science, IMS has initiated "Extreme Photonics" program in close collaboration with RIKEN and launched "Consortium for Photon Science and Technology (C-PhoST)" in cooperation with Osaka University, Kyoto University, and Japan Atomic Energy Agency. These programs have been endeavoring

to creating novel coherent light sources and utilizing them to detailed understanding and precise controlling of microscopic nature of materials. In addition, the UVSOR facility has been cooperating with Nagoya University and Kyoto University in "Quantum Beam Technology Program," to develop innovative synchrotron light sources with broader application.

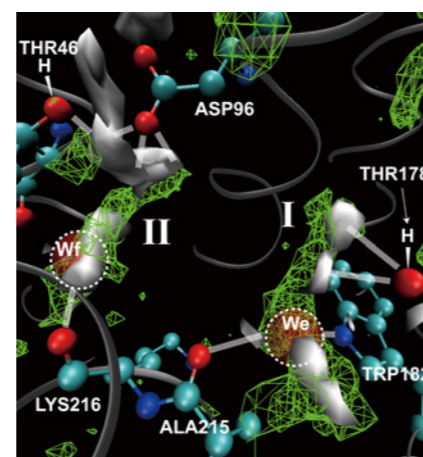


Experiment on Attosecond Coherent Control.



A snapshot of a symposium organized by C-PhoST.

In the field of theoretical and computational molecular science, IMS has been participating in "High Performance Computing Infrastructure (HPCI)" program of the nation. This program sets its strategic target as "Computational material science: Turning the headwaters of basic science into a torrent of innovations in functional materials and energy conversion," and endeavors the full utilization of the "K-computer," a next-generation supercomputer. Under the strategic program, IMS has set up the "Theoretical and Computational Chemistry Initiative (TCCI)," in close collaboration with the Institute for Solid State Physics, the University of Tokyo, and Institute for Material Research, Tohoku University, with the aim of significantly contributing in the field of material science and providing solutions to energy resources problems.



A comparison between the calculation results with MC-MOZ method, and that of an experiment, in one of the research themes, "fluctuation and dynamics in a condensed molecular science system."

### 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).

### Constructing a World-wide Research Network

IMS has accepted many foreign scientists and hosted numerous international conferences since its establishment and is now universally recognized as a leading institute that promotes firm international collaborations. In 2004, IMS initiated a new program to further promote international collaboration. As a part of this new program, IMS has been promoting the IMS International Internship Program for Foreign Graduate Students and the IMS International Fellowship Program for Young Foreign Researchers, through several foreign nominating institutions and universities. IMS has been also promoting the collaboration and exchange among IMS and core Asian institutions, ICCAS (China), KAIST (Korea), and IAMS (Taiwan), with a view to developing a new frontier in the molecular sciences and to foster the next generation of leading researchers, which was initially sponsored by JSPS Asian CORE Program (2006-2010) and succeeded as an IMS original program (2011-).

Visiting Foreign Researchers (2011)

Korea	33	Vietnam	2
Thailand	17	Ireland	1
France	17	Ukraine	1
China	17	Singapore	1
USA	15	Switzerland	1
India	12	Czech Republic	1
Germany	7	Norway	1
Taiwan	4	Bangladesh	1
UK	2	Poland	1
Australia	2	Malaysia	1
Canada	2	Lithuania	1
Turkey	2		

Total 142

## 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.

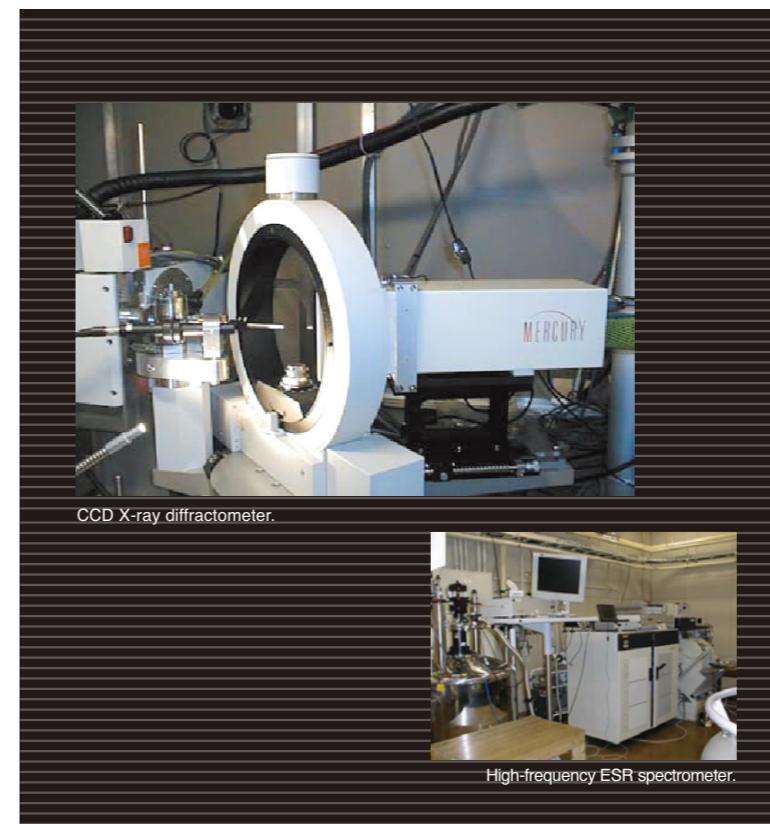
The university is based in Hayama, Kanagawa Prefecture, Japan, and its unique education programs are currently available in Hayama, as well as at eighteen other national academic research institutes to which individual students are assigned according to their fields of studies.

SOKENDAI Hayama Campus.



### UVSOR Facility

Light is called with various names such as infrared, visible, ultraviolet, vacuum-ultraviolet and X-ray, depending on its wavelength. A synchrotron light source is capable of producing light in the ultra-wide wavelength range from infrared to X-rays. Synchrotron light radiated by high energy electrons traveling in a strong magnetic field is intense and highly collimated. It is widely used in various research fields including molecular science. In IMS, a synchrotron light source has been operational since 1983. After several upgrades, it is still brightest in the world among low energy synchrotron light sources. By utilizing its excellent performance, the electronic structure that is the origin of the functionalities of solids is directly observed. This facility is called UVSOR and is used by many researchers not only from our country but also from foreign countries.

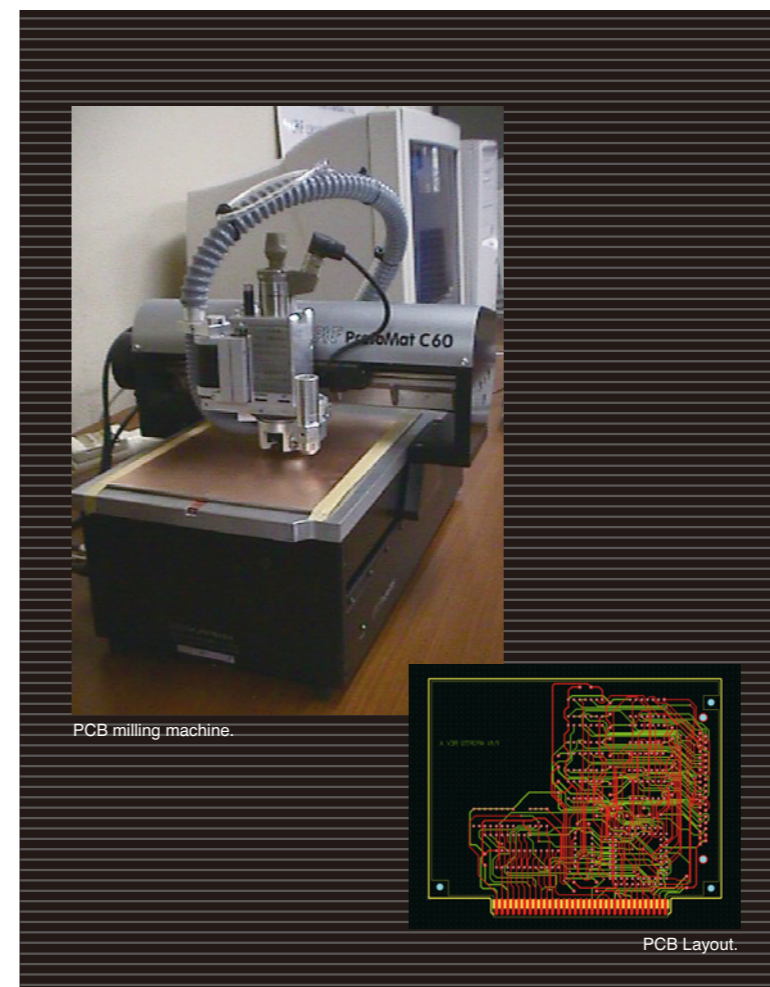
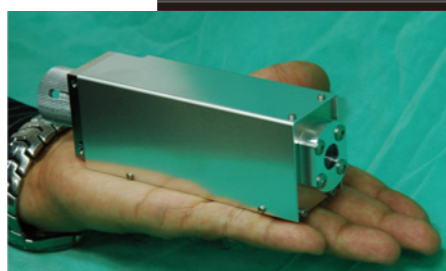
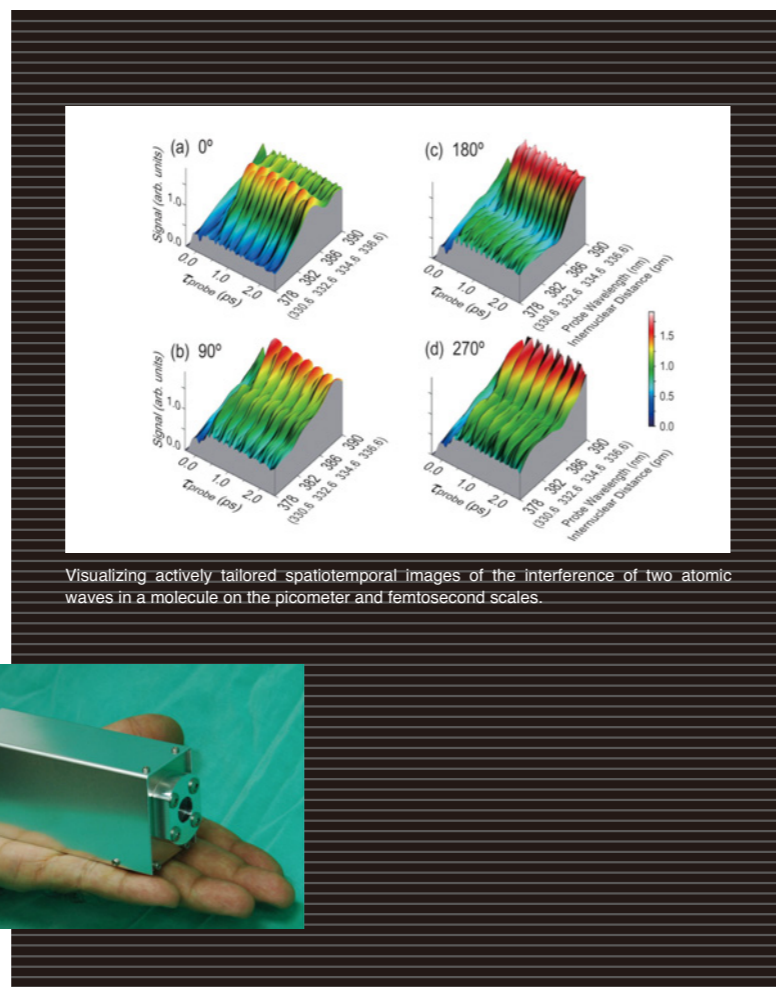


### Instrument Center

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 diffractometers, 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 experiment with combining lasers and general-purpose machines. We provide liquid nitrogen and liquid helium using helium liquefiers. We also support the inter-university network for common utilization of research equipments.

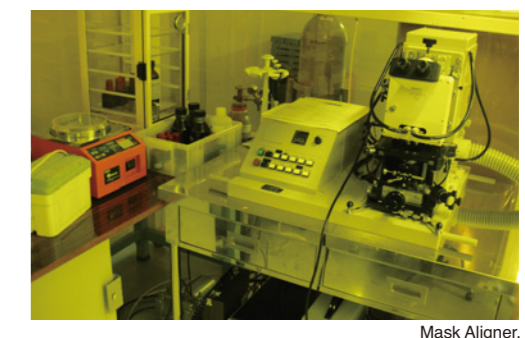
### Laser Research Center for Molecular Science

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.



### Equipment Development Center

We are developing various kinds of apparatus and devices required for conducting molecular science experiments. Facilities for machining, electronics and micro processing are in operation and engineers with technical skills of the highest level are in work. We have been developing various experimental apparatus since the establishment of IMS, in collaboration with in-house and outside scientists. We continue efforts for acquiring more advanced technical skills. We train scientists and students in short courses on machining and electronics.



### 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 300 TFLOPS.



Super-High-Performance Molecular Simulator.

### 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.

### 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]

◎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. On September 2010, the new dormitory called "Myodaiji lodge" opened at the Myodaiji area. This dormitory is for long stay.

#### Senior Scientific Advisors

YANAGIDA, Toshio Professor, Graduate School of Frontier Biosciences, Osaka University  
Graham R. Fleming Professor, University of California, Berkeley

#### Foreign Councilors

Ian A. Walmsley Professor, University of Oxford  
Thomas V. O'Halloran Professor, Northwestern University

#### Councilors

SAITO, Gunzi Professor, University of Meijo  
HIROTA, Noboru Professor, University of Kyoto  
MASUHARA, Hiroshi Professor, National Chiao Tung University

#### Advisory Committee

ASAKURA, Kiyotaka Professor, Catalysis Research Center, Hokkaido University  
KANDORI, Hideki Professor, Graduate School of Engineering, Nagoya Institute of Technology(Vice chair)  
KOHNO, Hirohiko Professor, Graduate School of Science, Tohoku University  
MIZUTANI, Yasuhisa Professor, Graduate School of Science, Osaka University  
MORI, Takehiko Professor, Graduate School of Science and Engineering, Tokyo Institute of Technology  
TERASAKI, Akira Professor, Faculty of Science, Kyushu University  
TSUKUDA, Tatsuya Professor, Graduate School of Science, Tokyo University  
UEMURA, Daisuke Professor, Faculty of Science, Kanagawa University  
YAMAGATA, Yuriko Professor, Graduate School of Pharmaceutical Science, Kumamoto University  
YAMANOUCI, Kaoru Professor, Graduate School of Science, Tokyo University  
AONO, Shigetoshi Professor, Okazaki Institute for Integrative Bioscience  
KATOH, Koichi Professor, Institute for Molecular Science  
KATOH, Masahiro Professor, Institute for Molecular Science  
KOSUGI, Nobuhiro Professor, Institute for Molecular Science(Chair)  
OHMORI, Kenji Professor, Institute for Molecular Science  
OHSHIMA, Yasuhiro Professor, Institute for Molecular Science  
OKAMOTO, Hiromi Professor, Institute for Molecular Science  
SAITO, Shinji Professor, Institute for Molecular Science  
UOZUMI, Yasuhiro Professor, Institute for Molecular Science  
YAMAMOTO, Hiroshi Professor, Institute for Molecular Science  
YOKOYAMA, Toshihiko Professor, Institute for Molecular Science

### Personnel and Budget

#### Staff (as of April, 2013)

Director-General	1
Professors	15 (9)
Associate Professors	17 (7)
Assistant Professors	38
Technical Staffs	35 (1)
Total	106 (17)

( ) Indicates the number of adjunct professors excluded.

#### Budget (FY 2012) (Thousand yen)

Personnel	1,126,099
Research	2,133,268
Facility	31,269
Total	3,290,636

#### Grants-in-Aid (FY 2012)\*

Grant-in-Aid Scientific Research (KAKENHI, MEXT and JSPS)**	335,157
Joint Research	40,525
from JST***	292,972
from MEXT***	161,112
Others***	427,577
Total	1,257,343

\* 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  
J S T : Japan Science and Technology Agency