

Department of Chemistry

Introduction

Chemistry is a science dealing with the structure, synthesis, and properties of substances, particularly at the molecular level. We are surrounded by chemical products; e.g., food, clothing, housing, drugs, and so on. In addition, new materials such as those supporting computer memory storage and superconductivity have been playing an essential role in the recent progress of technology and culture. Some chemicals, on the other hand, tend to give rise to serious environmental problems, whose solutions will depend upon chemistry research and education in future. Thus, chemistry and related sciences are much closer to us than one imagines, extensively contributing to the development of science and human society.

The department of chemistry, graduate school of science, Osaka University, comprises the following four divisions covering inorganic, physical, organic, and interdisciplinary chemistry. In addition, the department has cooperative with thirteen research groups of other research institutes.



Experiment in inorganic chemistry



Single Crystal growth of exotic organic functional materials under the oxygen-free condition (< 5 ppm)

Inorganic Chemistry Division

Analytical Chemistry, Inorganic Chemistry, Coordination Chemistry and Radiochemistry laboratories are included in this division.

Analytical Chemistry laboratory is developing nano-chemistry of liquid-liquid interfaces to elucidate specific role of the interface in chemistry. The diffusion dynamics of single molecules and the reaction mechanisms of metal-complex aggregations at the interface are investigated in relation to the separation mechanisms. New principles for migration analysis of biological micro-particles are also developed utilizing specific forces generated by a laser, an electric field and a magnetic field.

The main subject in both laboratories of Inorganic Chemistry is to explore novel transition metal complexes showing unique structures and properties. Various new types of mononuclear and polynuclear metal complexes have been synthesized and the relationship between their structures and chemical properties is elucidated in solid and solution states by means of electronic spectroscopy, NMR, X-ray diffraction and magnetic measurements. Furthermore, new spectroscopic phenomena induced by a magnetic field are also investigated.

In the Radiochemistry laboratory, superheavy elements and actinide elements are synthesized and their chemical properties are studied by some unique techniques. A new chemistry on artificial atoms composed of pion and muon, called an exotic atom, is developed in this laboratory. Nuclear reaction mechanisms of heavy ions and a finding of new nuclear phenomena, together with their application to physical and chemical researches, are also of their subjects.

In the Laboratory for bioinorganic chemistry, they study on relationships between structures and functions of metalloproteins, playing important roles in the biological systems. Furthermore, metal complexes are synthesized as a biomimetic model compound of the active site of metalloproteins, and the model complexes are structurally and functionally compared with the active site of proteins.



Synthetic organic experiment using exhaust equipment for safety

Physical Chemistry Division

In the physical chemistry division, our research and educational activities cover experimental studies of structure, properties and reactivity of molecules and condensed matter and their theoretical analysis.

In the Condensed Matter Physical Chemistry Group, electronic properties of molecular conductors, molecular magnets, metal complexes and their network magnetic systems are studied by calorimetry, transport, and magnetic measurements. Novel features originated from the cooperative effects of spins, charges and molecular motions are discussed.

The Surface Chemistry Group is concerned with electronic properties of molecules adsorbed on solid surfaces by means of fs-laser and electron spectroscopy. Micro-spot two-photon photoemission spectroscopy has been developed to probe unoccupied states in energy, time, and spatial domains.

Chemical Kinetics and Dynamics Group aims at understanding chemical reactions at single molecule or nano-level using novel methods of scanning probe microscopy. The investigation for devices consisting of small number of molecules based on single molecular reaction and/or properties develops novel features differing from that of bulk molecular materials.

Biophysical Chemistry Group maintains as its primary focus the development and use of laser-based technologies to measure atomic level features of the biological systems. The results of these efforts are contributing to a deeper understanding of the nature of proteins' motions and relating the dynamics to biological function.

In the Quantum and Theoretical Chemistry Group, Computers are utilized for theoretical analysis and prediction of properties and reactivity of chemical substances, design of functional materials. Development of new methodologies for computation is also the subject in this group.

The Research Center for Structural Thermodynamics is devoted specifically to chemical thermodynamics dealing with various types of condensed matter, including hard materials such as high- T_c superconductors, soft materials such as liquid crystals, and rather complex systems such as adsorbed monolayers. We are particularly interested in "Order and Disorder" created by subtle balance of various intermolecular interactions.

A physical chemistry group in the Museum of Osaka University is mainly working on the structure and dynamics of molecules confined in the nano-space constructed in the solid-state materials, by means of high-resolution solid-state NMR and ESR with other physico-chemical measurements. We also aim to develop a new analytical method for the cultural properties in Osaka University.

The Advanced Research System Development Group mainly focuses on surface chemistry explored with newly developed original experimental techniques and their related equipment. Particularly, the group is developing molecular-beam and ion-beam facilities for the studies of the elementary processes of surface-chemical reactions and of the surface modification including sputtering.

Organic Chemistry Division

In the Division of Organic Chemistry, we observe natural phenomena through the structures and chemical behaviors of organic molecules, and try to discover the underlying principles operating in the life systems. We also actively extend our knowledge through theoretical considerations of the structures and properties of molecules and molecular interactions. These efforts will allow us to interpretate the sophisticated natural system and enable further creation of functionally interesting organic compounds. Division of Organic Chemistry consists of the following four independent research groups.

The research in Laboratory for Physical Organic Chemistry is directed toward molecular design and synthesis of artificial novel compounds with theoretical and functional interests in the solid state properties. Such efforts may lead to an ultimate goal to realize self-organized single molecular electronics. Major research projects of Laboratory for Structural Organic Chemistry are related to synthesis of novel extended π -electron systems and artificial supramolecules. New synthetic procedures for molecules with conjugated electronic systems are also investigated there. Systematic studies of properties for such various synthetic compounds are expected to result in discovery of novel classes of functionally interesting and versatile compounds.

Laboratory for Natural Products Chemistry mainly focuses on the functions of glycoconjugates consisting of carbohydrates linked to other structural units such as fatty acids and phosphates. Isolation of unknown bioactive compounds from natural sources, their structural, synthetic and functional studies are being intensively undertaken. The research purpose in Laboratory for Organic Biochemistry is to clarify the functions of oligosaccharides in the living cell. Chemical synthesis of glycoproteins, glycopeptides and oligosaccharides are potentially performed and then used it for several bioassays in order to elucidate oligosaccharide functions. Several new reactions to construct such biomolecular are also studied.

Interdisciplinary Chemistry Division

In this Division research works are oriented towards novel fields of both bioorganic and bioinorganic chemistry. Marine toxins and other biologically active compounds such as lipids and hormones are dealt with in Laboratory for Biomolecular Chemistry. New methodologies based mainly on NMR spectroscopy are being elaborated for investigation of three-dimensional structures and functions of complex biomolecules. The purpose of Laboratory of Coordination Chemistry is to prepare novel mononuclear, polynuclear, and metallosupramolecular complexes and to elucidate their molecular structures, electronic states, and functionalities. In particular, our current interest is directed toward the development of fundamental coordination chemistry by utilizing multifunctional metalloligands instead of classical inorganic/organic ligands.

Research Projects

Inorganic Chemistry Division

1. Laboratory for Analytical Chemistry
2. Laboratory for Radiochemistry
3. Laboratory for Inorganic Chemistry
4. Laboratory for Bioinorganic Chemistry

Physical Chemistry Division

5. Laboratory for Condensed Matter Physical Chemistry
 6. Laboratory for Surface Chemistry
 7. Laboratory for Quantum Chemistry
 8. Laboratory for Reaction Dynamics
 9. Laboratory for Biophysical Chemistry
- Advanced Research System Development Group

Organic Chemistry Division

10. Laboratory for Structural Organic Chemistry
11. Laboratory for Physical Organic Chemistry
12. Laboratory for Natural Product Chemistry
13. Laboratory for Organic Biochemistry

Interdisciplinary Chemistry Division

14. Laboratory for Biomolecular Chemistry
15. Laboratory for Coordination Chemistry
16. Research Center for Structural Thermodynamics
17. Laboratory for High-Technology Research for the Analysis and Utilization of Materials

18. Center for Education in Liberal Arts and Sciences
19. Radio Isotope Research Center

The Institute of Scientific and Industrial Research (Cooperative Division)

20. Laboratory for Semiconductor Materials and Processes
21. Laboratory for Bio-Nanotechnology
22. Laboratory for Regulatory Bioorganic Chemistry
23. Laboratory for Synthetic Organic Chemistry

Institute for Protein Research (Cooperative Division)

24. Laboratory of Protein Organic Chemistry
25. Laboratory for Molecular Biophysics
26. Laboratory of Protein Profiling and Functional Proteomics

Cooperative Adjunct Division

27. National Institute of Advanced Industrial Science and Technology (AIST) Inorganic Functional Materials Research Institute
28. National Institute of Advanced Industrial Science and Technology (AIST) Inorganic Functional Materials Research Institute
29. National Institute of Advanced Industrial Science and Technology (AIST) Research Institute of Electrochemical Energy
30. Peptide Institute, Inc.
31. Suntory Foundation for Life Sciences, Bioorganic Research Institute

Department
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Laboratory for Analytical Chemistry

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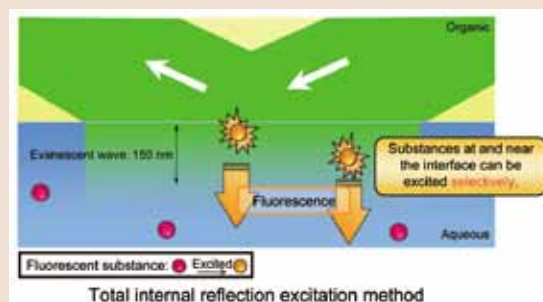
Home Page <http://www.chem.sci.osaka-u.ac.jp/lab/tsukahara/en/index.html>

[Research Interests]

- 1) Metal complex aggregation at liquid/liquid interfaces and its high sensitive spectroscopic analysis
- 2) Measurements and analysis of denaturation of proteins at hydrophobic interfaces
- 3) Measurements of transport kinetics of substances through liquid/liquid interfaces and development of high selective interfaces
- 4) Development of magneto-optical microscope under pulsed magnetic field
- 5) Development of analytical separation methods for microparticles exploiting external field
- 6) Structural analysis of chiral molecules in solutions based on Raman optical activity spectroscopy

Measurements of chemical reactions and phenomena occurring at liquid/liquid interfaces and analysis of nanoparticles and microparticles relating to biological and environmental systems are much important and attractive subjects in Analytical Chemistry. We have invented new methods to measure absorption spectra of metal complex aggregates

formed at liquid/liquid interfaces with polarized light; the thickness of the aggregates is only a few nanometers. We also measured reversible adsorption of proteins to hydrophobic interfaces by total internal reflection technique, and investigated the denaturation of proteins there. We have also invented novel analytical methods for microparticles by using magnetic field. Magneto-optical imaging microscopy and analytical separation method are being developed in order to detect paramagnetic compounds in microparticles.



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Laboratory for Radiochemistry

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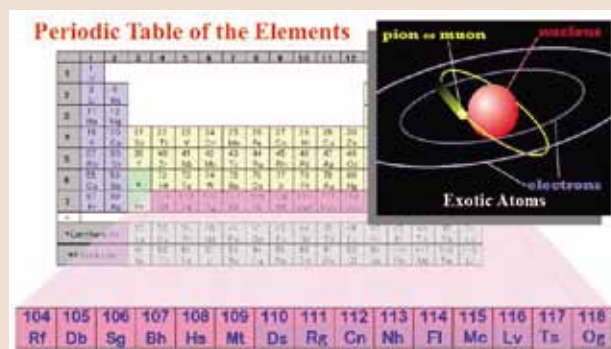
[Research Area]

- 1) Chemistry of superheavy elements
- 2) Chemistry of exotic atoms
- 3) Preparation of radionuclides for medical use, Environmental radioactivity, Chemistry related with radioactive elements and nuclear properties

Chemistry of superheavy elements: The chemistry of transactinide elements – which can also be termed superheavy elements – has now reached element 108. We have been studying the chemical properties of heavy-actinide and transactinide elements. Our interests have concentrated on the question how well the Periodic Table of the Elements accommodates the transactinide elements as transition metals in the 7th period. Development of apparatus for “single atom chemistry” and the related tracer experiment are also making progress for the project above.

Chemistry of exotic atoms: The goal of this theme lies in

comprehensively understanding the formation mechanism and behavior of pionic/muonic atoms and molecules in order to apply the phenomenon to analytical chemistry and material science, and to develop a new chemistry of the 2nd generation substance.

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Laboratory for Inorganic Chemistry

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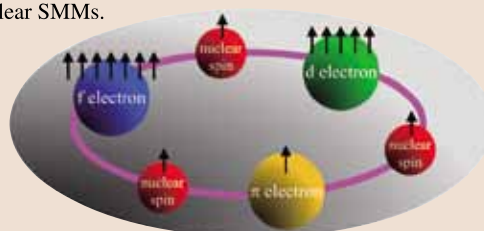
Home Page http://www.chem.sci.osaka-u.ac.jp/lab/ishikawa/english_welcome.html

[Research Interests]

- 1) Electronic structure and molecular magnetism of the systems containing 4f electrons
- 2) New molecular devices such as single-4f-ionic single molecule magnets
- 3) Time-domain behavior of quantum states of the systems containing multiple single molecule magnets
- 4) Chemical and physical manipulation of ligand field potential, magnetic anisotropy and molecular magnetism

“Metal complexes” and “supramolecules” can contain unpaired electrons of several different kinds. The unpaired electrons have magnetic moments which are responsible for various intriguing magnetic properties. Atomic nuclei also have magnetic moments whose strength varies from nucleus to nucleus. Such magnetic moments interact to construct complicated quantum states. One of our research aims is to understand such quantum states through experimental and theoretical analysis. For some unsolved

problems, such as sub-structure of the ground states of lanthanide complexes having 4f-electronic systems, we develop computational tools to solve them. Solving such unsolved problems some times leads to discovery of new properties of molecules. One of such properties is the “Single Molecule Magnet (SMM)” behavior of mono-nuclear lanthanide-phthalocyanine complexes, which had been considered possible only for polynuclear metal complexes. At present the lanthanide-phthalocyanine complexes are regarded as the most promising SMMs for future applications. Our research target has been extended to understanding and controlling of time-domain behavior of 4f-electronic systems, including mono- and multiple-nuclear SMMs.



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Laboratory for Bioinorganic Chemistry

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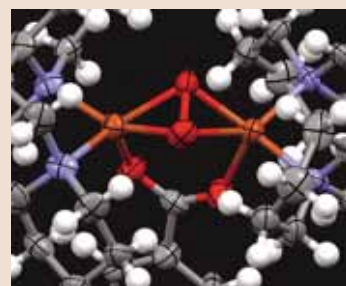
[Research Interests]

- 1) Dioxygen activation by model compounds mimicking the active sites of dicopper- and multicopper-containing enzymes
- 2) Synthesis of model compounds of the oxygen-evolving complex (OEC) in photosystem II
- 3) Synthesis of cage type metal complexes with an encapsulated photo-excitation unit
- 4) Synthesis of low-valent first-row transition metal complexes for activation of small molecules
- 5) Structural biology for elucidating functions of metalloproteins

The energy transduction and metabolic processes of biological systems involve photoexcitation, electron transfer, small molecule activation, etc. The active sites of the relevant proteins perform their functions in a limited cavity of the large protein structure. Focusing on the important roles of the active metal site and the surrounding protein structure, we are investigating

the metalloproteins with a multi-spherical structure formed by the protein molecules and their synthetic model compounds specifically designed for the active metal sites in order to gain insights into the essence of their reaction mechanism.

We study metalloproteins containing copper or iron centers at the active site mainly on the basis of X-ray crystal structure analysis. As a further step toward understanding of the transition metal centers at the active site, we design and synthesize their structural and reaction model compounds to clarify the structure-reactivity relationship.



Structure of a dicopper-dioxygen adduct complex

Department
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Chemistry

Laboratory for Condensed Matter Physical Chemistry

Members Yasuhiro NAKAZAWA (Professor), Hiroki AKUTSU (Associate Professor)
Satoshi YAMASHITA (Assistant Professor)

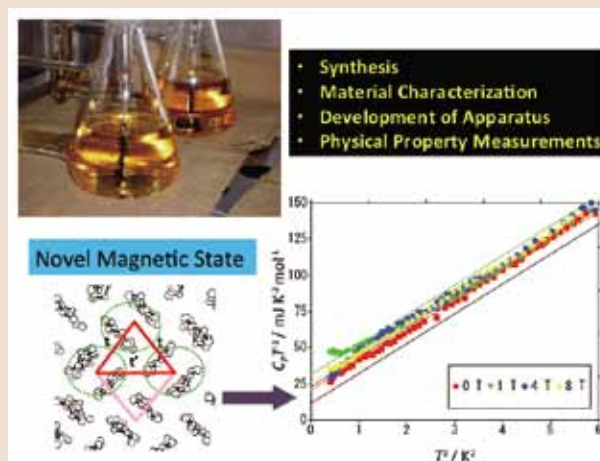
Home Page <http://www.chem.sci.osaka-u.ac.jp/lab/nakazawa/>

[Research Area]

- 1) Phase Transitions and Low-Energy Excitations in Molecular Superconductors.
- 2) Novel Quantum Behavior in Strongly Correlated Electron Systems.
- 3) Magnetic Behaviors of Molecular Magnets and Metal Complexes.
- 4) Search for Novel Quantum Phenomena under Various External Conditions.

We are studying the physical and chemical properties of condensed matter systems which consist of molecules and atoms. Especially we are interested in finding novel phenomena and their possible mechanisms with regard to superconductivity and magnetism. Along this line, we have constructed our original low-temperature calorimeters for measuring heat capacities of small single-crystal samples. To see the behavior induced by changing the external condition, the calorimetry under external magnetic

fields up to 15 T is also performed. Throughout the thermodynamic research, we are aiming at solving the mechanisms of many mysterious behaviors in condensed matter systems.



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Laboratory for Surface Chemistry

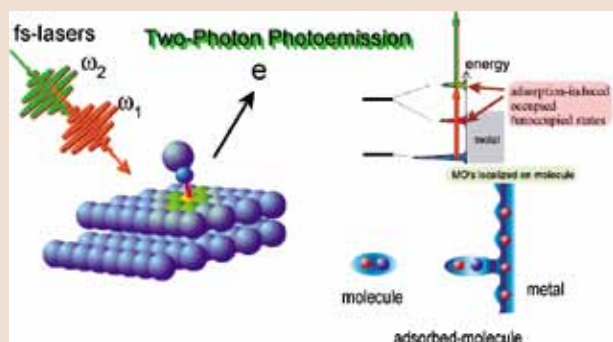
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[Research Interests]

- (1) Photoemission microscopy for organic films
- (2) Electronically excited states of adsorbed molecules



[Research Area]

Unoccupied electronic states play crucial roles in functionality and chemical reactions at surfaces. We are concerned with spectroscopy and dynamics of the unoccupied states by means of two-photon photoemission (2PPE) spectroscopy. Upon adsorption of molecules on a surface, adsorption-induced occupied and unoccupied states are formed in the vicinity of the Fermi level. The adsorption-induced states are probed with 2PPE spectroscopy providing insights on chemical properties of surfaces covered with molecules. A microbeam photoemission spectrometer was developed by use of coherent radiation at a wavelength of 140 nm. The micro-spectrometer, which achieved an energy resolution of 30 meV and a lateral resolution of 0.3 μm , is applied to reveal lateral inhomogeneity of electronic structures of organic films.

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Laboratory for Quantum Chemistry

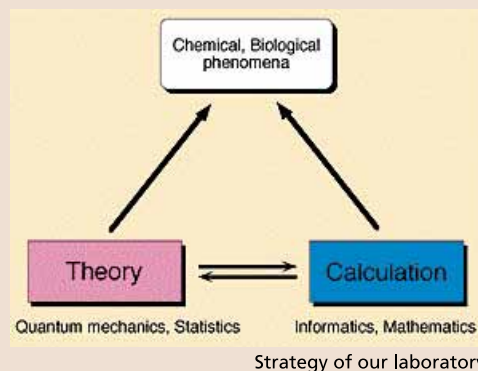
Members Mitsutaka OKUMURA (Professor), Shusuke YAMANAKA (Associate Professor), Takashi KAWAKAMI (Assistant Professor)

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[Research Area]

- 1) Theoretical studies on molecular and electronic structures for atoms, molecules and their clusters.
- 2) Theoretical studies on chemical reaction.
- 3) Theoretical studies on electronic, magnetic and photo properties.
- 4) Theoretical studies on functional, informatics and mathematical systems.

In this laboratory the investigations depending on only theory and calculation are performed for many chemical subjects. We employ quantum mechanics, statistics and informatics as fundamental theory for investigation of electronic and molecular structures. Moreover, ab initio MO program packages based on our own theory are developed to challenge cluster, biological sciences and etc., which expand possibilities of chemical subjects. Accurate and huge calculations as well as visualization of their results using super-computers are also applied to the elucidation of intriguing chemical phenomena before experimental studies.



Department
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Chemistry

Laboratory for Reaction Dynamics

Members Takuya MATSUMOTO (Professor), Hiroshi OHYAMA (Associate Professor), Dock-Chil CHE (Associate Professor), Youichi OTSUKA (Assistant Professor)

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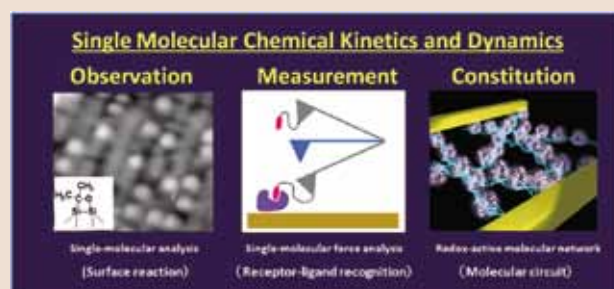
Home Page <http://www.chem.sci.osaka-u.ac.jp/lab/matsumoto/index.html>

[Research Interests]

- 1) Time-resolved electrostatic force microscopy for electron-transfer dynamics.
- 2) Molecular recognition force microscopy for receptor-ligand reaction.
- 3) Molecular electronics based on redox-active molecular array.
- 4) Multi-dimensional stereodynamics in the molecular-molecular reactions.
- 5) Stereodynamics in the molecular-radical reactions.

The chemistry of individual molecules has been a chemist's dream for long time, but today, it is realized by scanning probe microscopy. The method enables us to observe, measure, and manipulate individual molecules in nano-scale. We are studying molecular recognition and electron transfer using scanning probe microscopy in single molecule level, and interested in finding novel phenomena which differ from those of bulk molecular materials. Along this line, the devices consisting of small number

of molecules are also developed from a perspective of molecular electronics.

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Laboratory for Biophysical Chemistry

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[Research Area]

- 1) Structural chemistry on allosteric proteins.
- 2) Energy flow in proteins.
- 3) Allostery and functionality of proteins.
- 4) Development of techniques for time-resolved spectroscopy.

Our research focuses on functionally-important protein dynamics to elucidate mechanism how they function. Protein dynamics are intimately connected to the structure/function relationship of biological systems. In numerous biological processes, the ensuing protein structural changes accompanying a reaction at a specific site must spatially extend to the mesoscopic dimensions of the protein to achieve a biological function. Protein dynamics span over a wide range of time scales. To answer questions on protein dynamics, we need the concatenation of experimental results recorded over many orders of magnitude of time. In this regard it is important that a single experimental technique can examine protein structures evolving from the earliest moments, such as the picosecond regime, toward time scales that

are highly relevant to biological functions, such as the microsecond or millisecond regimes. We are studying protein dynamics in the wide time window by using various time-resolved spectroscopic techniques, such as resonance Raman, absorption, and fluorescence spectroscopy.



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Advanced Research System Development Group

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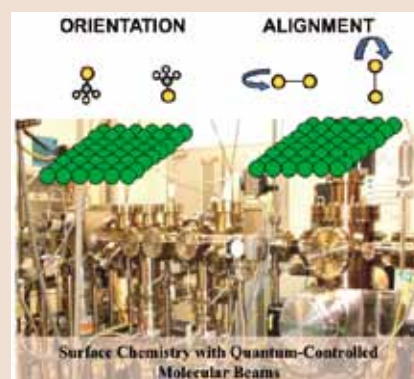
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[Research Interests]

- 1) Stereodynamics of surface chemical reactions induced by molecular beams
- 2) Surface chemical reactions explored with various surface-spectroscopy techniques
- 3) X-ray photoemission spectroscopy at SPring-8 for surface chemistry
- 4) Surface phase transition induced by the low dimensionality
- 5) Tuning of surface reactivity with surface alloying
- 6) Development of new type of secondary ion mass spectroscopy with very low-energy ions

Advanced Research System Development Group mainly focuses on surface chemistry explored with newly developed original experimental techniques and their related equipments. Particularly, the group is developing molecular-beam and ion-beam facilities for the studies of the elementary processes of

surface-chemical reactions and of the surface modification including sputtering.

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Chemistry

Laboratory for Structural Organic Chemistry

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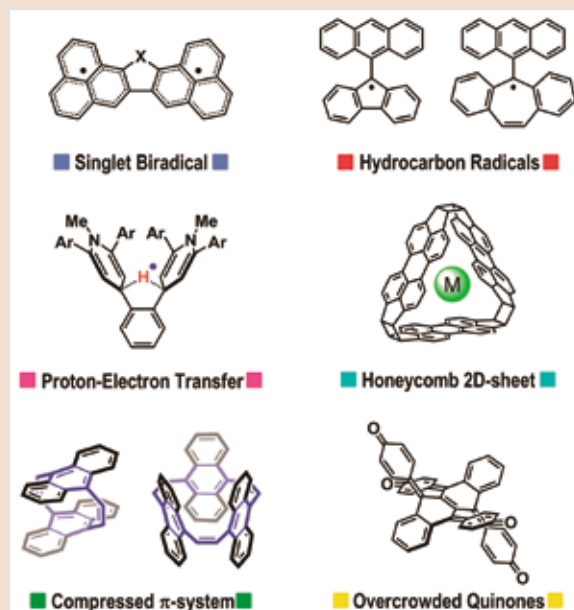
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[Research Interests]

- 1) Synthesis and solid-state properties of open-shell molecules
- 2) Development of proton and electron transfer system
- 3) Design, synthesis, and properties of molecular-based 2D-sheet materials
- 4) Synthesis and functions of π -compressed molecules
- 5) Synthesis, structures, and properties of overcrowded quinones

π -Electrons in conjugated molecules play decisive roles for the electronic and photo-physical properties of organic compounds. We have been studying designs, syntheses, structures, and physical properties of novel extended π -conjugated systems, with particular emphasis on functional properties such as electron-transport, magnetism, supramolecular chemistry, photo-switching, and chiro-optics. Work in these areas is highly synthesis-driven, and is also strongly based on physical organic chemistry. Our wide variety of chemistry will lead to discovery of new class of electronic- and photonic-materials as well as of fundamental scientific ideas.



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Laboratory for Physical Organic Chemistry

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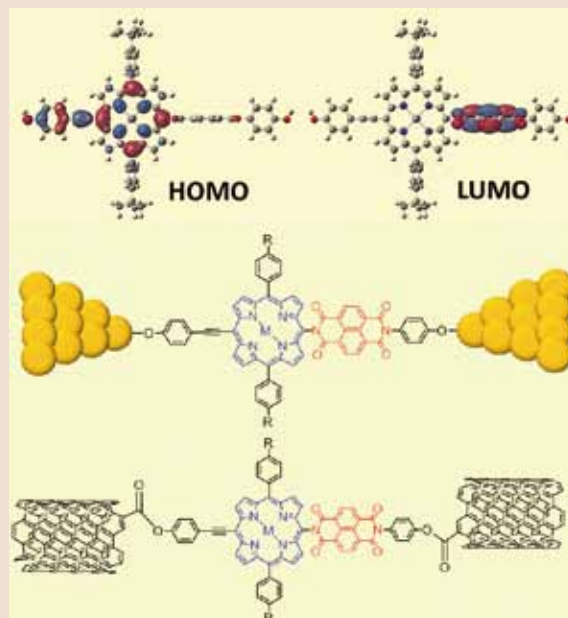
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[Research Interests]

- 1) Design, synthesis and measurement of molecules which have non-linear and non-symmetrical single molecule electronic properties.
- 2) Complexation of nano-carbon materials such as carbon nanotubes or graphene nano ribbons with organic molecules and study of their electronic properties.
- 3) Self-assembling of organic molecules on surfaces.
- 4) Development of novel magnetic molecules.

Molecular scale electronics are desirable fields not only for fundamental interest but also for applied aspects. We are working on synthesis of new conductive nanomaterials (carbon nanotubes, metal nanorods, and metal nanoparticles) and functional organic molecules. We are also developing new methodologies which enable us to explore these nanomaterials in molecular scale accuracy.

Department
of
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Laboratory for Natural Product Chemistry

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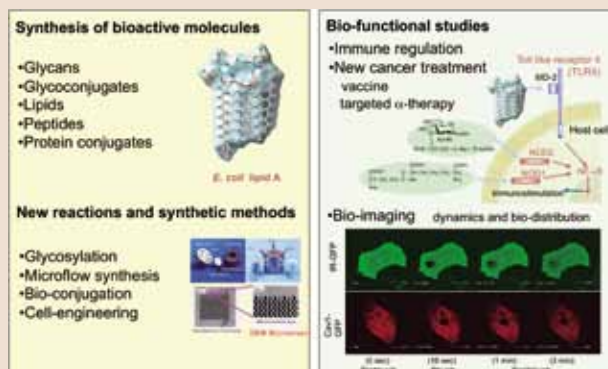
Home Page <http://www.chem.sci.osaka-u.ac.jp/lab/fukase/>

[Research Interests]

- 1) Chemistry and function of immunomodulating glycoconjugates
- 2) Efficient and selective methods for glycosylation and oligosaccharide synthesis
- 3) Bio-imaging of glycans and proteins for the new functional studies
- 4) Targeted a-radiation therapy for cancer

We have studied chemistry and biology of cell surface glycoconjugates of bacteria and mammals. Synthetic studies of bacterial immunostimulating glycoconjugates such as lipopolysaccharide (LPS) and peptidoglycan led to the identification of their active entities responsible for the primary defense mechanism of host animals against bacterial infection. Sensing receptors of the innate immunity have been identified and the receptor-ligand interactions have been elucidated by using our synthetic compounds. Stereoselective glycosylation reactions such as α -sialylation and β -mannosylation have been established in this laboratory. Biological functions of *N*-glycans on proteins have

been investigated by the chemical synthesis of complex oligosaccharides as well as by a new synthetic biology approach. Bio-imaging study of glycans, peptides, and proteins have been also investigated by using fluorescent microscopy. Novel methods for cancer treatments such as cancer vaccines and targeted α -radiation therapy are now important projects in our group.



Department
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Laboratory for Organic Biochemistry

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[Research Interests]

- 1) Chemical synthesis of oligosaccharides
- 2) Chemical synthesis of glycoproteins and glycopeptides
- 3) Elucidation of oligosaccharide functions

The oligosaccharides of protein have been thought to concern with protein conformation, dynamics, protein trafficking and glycoprotein lifetime in blood. We have examined synthesis of homogeneous glycoproteins having human complex type oligosaccharide in order to evaluate oligosaccharide functions. We have synthesized several small glycoproteins (amino acids 40-76 residues), erythropoietin analogue (amino acids 166 residues), and co-stimulate glycoprotein of T-cell (amino acids 120 residues). In order to synthesize these glycoproteins, the polypeptide sequence of target glycoprotein were divided into several segments and these were synthesized by solid phase peptide synthesis. After prepared both glycopeptide-thioester and peptide, these were coupled by repetitive Native Chemical Ligation (NCL). After construction of

the glycosylated polypeptide chain, we examined folding experiments and evaluated effect of oligosaccharide during protein folding process. In addition, glycoproteins folded was analyzed its structure by NMR and CD spectra in order to evaluate conformational differences between glycosylated and nonglycosylated proteins. In our laboratory, we would like to elucidate oligosaccharide functions by use of such chemical approach.

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Laboratory for Biomolecular Chemistry

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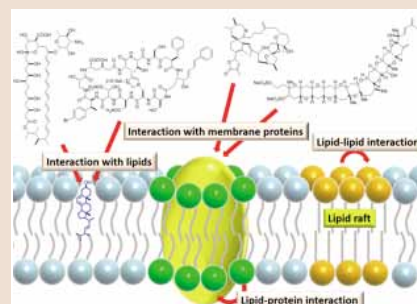
Home Page <http://www.chem.sci.osaka-u.ac.jp/lab/murata/english/index.html>

[Research Interests]

- 1) Structural analysis of the drug assembly at biological membranes
- 2) Complex structure and interaction analysis of bioactive lipids and proteins
- 3) Lipid assembly and molecular recognition mechanism at lipid rafts
- 4) Chemical synthesis and functional analysis of complex natural products

Natural products are a rich source of bioactive compounds. For the better understanding of their molecular mode of action, the precise 3D structures and dynamic behavior have to be elucidated. Our approach is based on solution/solid-state NMR spectroscopy in combination with organic synthesis. Bioactive molecules show their activity by binding with cell membrane or with transmembrane peptides, thereby forming a self-assembly

or complex. Our objectives are to solve the 3D structures of these molecular assemblage on the basis of NMR analysis with synthetically isotope-labeled compounds. We are currently trying to work out the structure of molecular assemblages by polyene antibiotics/membrane lipids. Our research focuses on bioactive compounds including drugs, toxins, and endogenous small molecules such as lipids, sterol, and peptides, particularly on their interactions with biomembranes.



Department
of
Chemistry

Laboratory for Coordination Chemistry

Members Takumi KONNO (Professor), Nobuto YOSHINARI (Associate Professor), Naoto KUWAMURA (Assistant Professor), Tatsuhiro KOJIMA (Assistant Professor)

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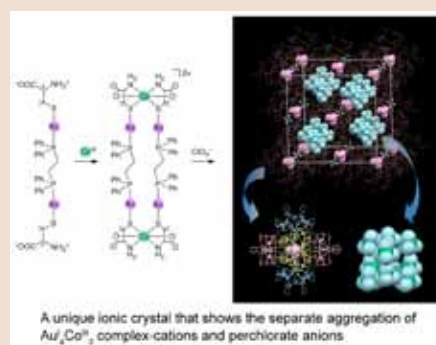
Home Page http://www.chem.sci.osaka-u.ac.jp/lab/konno/index_e.html

[Research Interests]

- 1) Exploitation of coordination molecular technology that leads to the creation of new conceptual ionic solids with new functionalities.
- 2) Stepwise construction of heterometallic polynuclear and metallosupramolecular structures based on multifunctional metalloligands.
- 3) Studies on the chiral recognition and self-assembly of metal complexes.
- 4) Studies on the control of structures and properties of sulfur-bridged polynuclear complexes.

The purpose of our research projects is to prepare novel mononuclear, polynuclear, and metallosupramolecular complexes and to elucidate their molecular structures, electronic states, and functionalities. In particular, our current interest is directed toward the development of fundamental coordination chemistry by utilizing multifunctional metalloligands instead of classical inorganic/organic ligands. Based on this strategy, we have been investigating the rational, stepwise, and chiral-selective

constructions of polynuclear and metallosupramolecular architectures by the use of simple organic compounds such as amino acids as a starting materials in combination with several kinds of transition metal ions, as well as the exploration of new coordination modes and oxidation states that are created in these unique heterometallic architectures. Recently, we succeeded in the creation of new ionic solids that consist of cationic aggregates and anionic aggregates.

Department
of
Chemistry

Research Center for Structural Thermodynamics

Members Motohiro NAKANO (Professor), Yuji MIYAZAKI (Associate Professor), Yatsuhisa NAGANO (Associate Professor), Daisuke TAKAJO (Assistant Professor)

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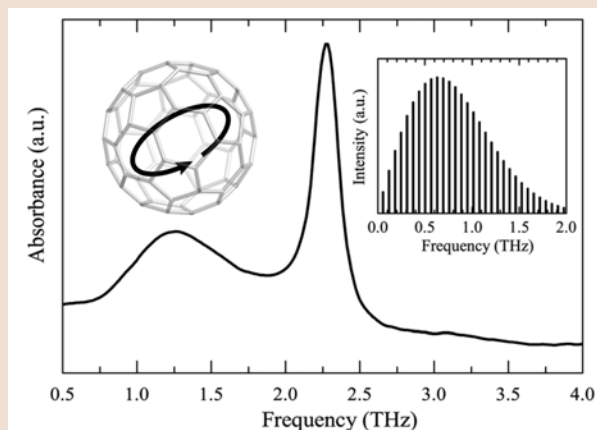
Home Page <http://www.chem.sci.osaka-u.ac.jp/lab/micro/index.html.en>

[Research Interests]

- 1) Thermodynamic investigation of molecule-based magnets.
- 2) Thermodynamic investigation on biomolecules and macromolecules in aqueous solutions.
- 3) Thermodynamic approach to biological phenomena.
- 4) Thermochemical approach to chemical bonds.
- 5) Structure and thermodynamics of molecular monolayers.
- 6) Characterization of solutions in terms of higher derivatives of thermodynamic potentials.

We are particularly interested in "Order and Disorder" created by subtle balance of various intermolecular interactions. Among many experimental techniques used in chemical science, our specialty is to measure the "Energy and Entropy" very accurately by means of calorimetry. Our goal is to combine all the information obtained from both the microscopic and macroscopic investigations to uncover the nature of condensed matter, which leads us to harmonize "molecular" sciences and chemical

"thermodynamics". Applicability of thermodynamics allows us to target at hard samples including metals, ceramics, and molecular crystals in addition to soft ones like biopolymers, solutions, monolayers, and living things.



Rotational band of Li cation encapsulated in C60 cage by THz spectroscopy.

Department
of
Chemistry

Laboratory for High-Technology Research for the Analysis and Utilization of Materials

(The Museum of Osaka University)

Members Takahiro UEDA (Professor), Jiro TOYODA (Associate Professor),
Keisuke MIYAKUBO (Associate Professor)

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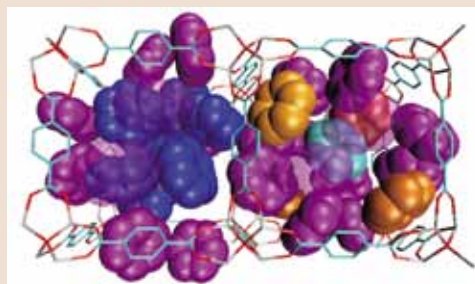
Home Page <http://www.museum.osaka-u.ac.jp/chemistry/index-jp.html>

[Research Interests]

- 1) Physicochemical properties and intermolecular interactions of guest molecules confined in nanospace
- 2) Construction of new molecular assembly using a uniquely restricted nanospace and investigation of their novel properties
- 3) Development of new porosimetry based on NMR spectroscopy
- 4) Development of a new analytical method for the cultural properties using magnetic resonance spectroscopy
- 5) Construction of the Database for the Museum of Osaka University

Our laboratory is working on the structure and dynamics of molecules confined in nano space constructed in the solid-state materials, by means of state-of-the-art high-resolution solid-state NMR spectroscopy with other physico-chemical measurements. We also examine the new molecular assembly using a uniquely restricted nanospace and investigate their novel properties.

Furthermore, we also aim to develop a new analytical method for the cultural properties using NMR spectroscopy, as well as to construct a database and develop a network system for the exchange of information about the primary materials in Osaka University.



The local structure of benzene confined in Zn-based porous coordination polymer, IRMOF-1, obtained by molecular dynamics simulation.

Department
of
Chemistry

Center for Education in Liberal Arts and Sciences

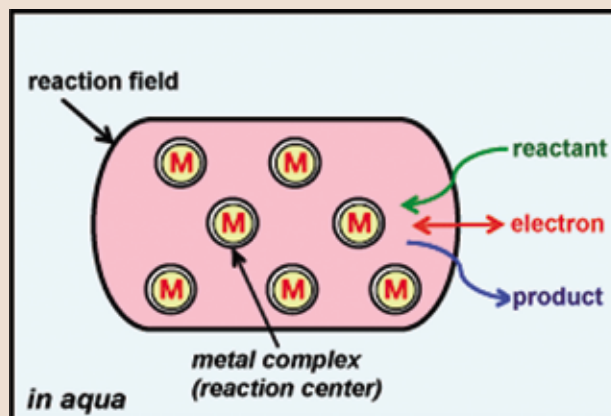
Members Kazuya YAMAGUCHI (Professor)

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[Research Interests]

- 1) Effect of reaction field on the function of model complexes for the active site of metalloenzyme
- 2) Function conversion of dinuclear metalloenzymes
- 3) Preparation of new functional materials with biological metal complexes

Metal ions play important roles to maintain structures and functions in biological systems. Our current works are focused on (1) studies of structures and functions of metal proteins (Cu, Ni, Fe etc.) by various spectroscopy, and (2) syntheses and structural and functional characterization of transition metal complexes as models for the active sites of metalloproteins. Specially, we investigate the effect of reaction field on the function of metal complexes. Moreover, we challenge the function conversion of metalloenzyme with the metal ion substitution and recombinant DNA methods. We believe that the studies will give the important information for preparation of new functional materials with biological metal complexes.



Department
of
Chemistry

Radioisotope Research Center

Members Takashi YOSHIMURA (Professor), Kojiro NAGATA (Assistant Professor)

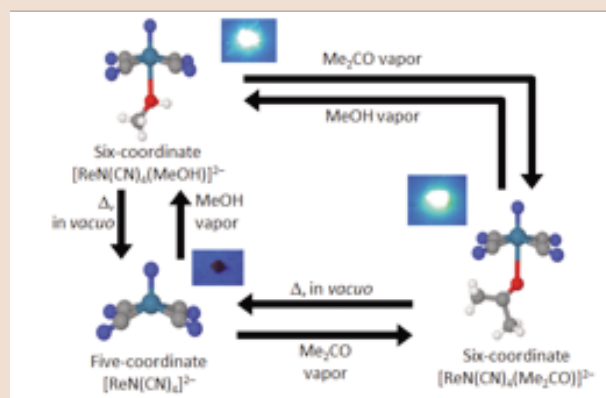
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Home Page <http://www.rirc.osaka-u.ac.jp/yoshimura/>

[Research Interests]

- 1) Synthesis and properties of uranium complexes
- 2) Separation and structural studies of actinides and lanthanides
- 3) Synthesis and photoluminescent properties of metal complexes

Radioactive elements account for nearly a quarter of the elements of the periodic table. In order to elucidate the periodic law of the elements in more detail, knowledge of the chemistry of radioactive elements is important. Recent our research project is to synthesize new uranium complexes. It is interesting to separate trivalent actinides and lanthanides because the chemical properties are very similar. We have studied about synthesis of new chelating ligands to separate them and structural properties of the lanthanides complexes. Moreover, we are interested in synthesis of new photoluminescent metal complexes.

Department
of
Chemistry

Laboratory for Semiconductor Materials and Processes (The Institute of Scientific and Industrial Research)

Members Hikaru KOBAYASHI (Professor), Taketoshi MATSUMOTO (Associate Professor), Kentaro IMAMURA (Assistant Professor)

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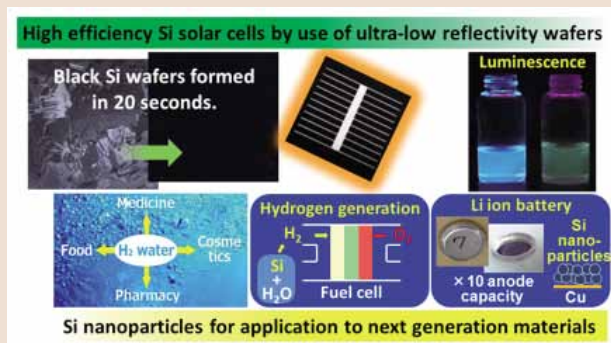
[Research Interests]

- 1) High efficiency Si solar cells by use of new chemical methods.
- 2) Si nanoparticles for application to next generation energy materials.
- 3) Observation of semiconductor interface states by use of a new spectroscopic method.

We are studying materials, devices and processes relating with semiconductors, especially, silicon and silicon nanoparticles. Our goal is application of our fundamental results to society.

Although theoretical limit of energy conversion efficiency for silicon solar cells is about 30%, energy conversion efficiencies of commercial silicon solar cells are only 15~18% due to reflection at Si surfaces and recombination of electrons and holes at defects. New chemical methods to prevent reflection at Si surfaces and recombination of electrons and holes have been developed to overcome these issues.

Silicon nanoparticles possess wide band-gaps due to the quantum size effect and high activity for surface reaction. Light emitting materials and hydrogen source by reaction with water and anode active materials for lithium ion batteries have been developed with silicon swarf. We are also studying effects of the hydrogen-containing water on human body.



Department
of
Chemistry

Laboratory for Bio-Nanotechnology

(The Institute of Scientific and Industrial Research)

Members Masateru TANIGUCHI (Professor), Makusu TSUTSUI (Associate Professor),
Hiroyuki TANAKA (Assistant Professor), Kazumichi YOKOTA (Assistant Professor)

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[Research Interests]

- 1) Electrical and thermal properties in single-molecule junctions
- 2) Single-molecule electrical sequencing of DNA, RNA, and peptide based on quantum chemistry
- 3) Single-molecule fluid dynamics and its controlling method
- 4) Single-molecule observations with atomic resolutions

We are challenging biology through the development and use of single-molecule science and technology based on chemical physics. In an effort to explore single-molecule science, we are studying electrical and thermal properties of single-molecule junctions formed by metal electrodes and single molecules. In addition, we are attempting to elucidate biological behaviors using quantum-chemistry-based, single-molecule electrical sequencing of DNA, RNA, and peptides because the central dogma of molecular biology explains the genetic information flow within a biological system. Moreover, we are investigating single-molecule fluid dynamics in solutions and developing methods for controlling

fluid dynamics because biomolecules exist and function in the solutions. Furthermore, to better understand single-molecule behaviors deduced from electrical measurements, we observe single molecules at atomic resolutions using optical and scanning tunneling microscopes. Our primary goal is to develop single-molecule science and technologies, which are expected to revolutionize molecular biology, medical sciences, and drug development.

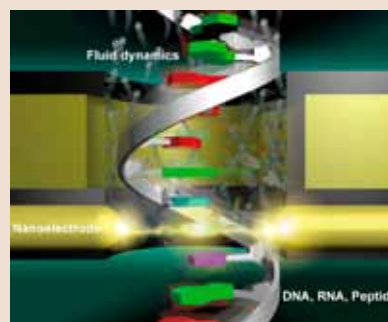


Fig. Schematic of single-molecule sequencing method.

Department
of
Chemistry

Laboratory for Regulatory Bioorganic Chemistry

(The Institute of Scientific and Industrial Research)

Members Kazuhiko NAKATANI (Professor), Chikara DOHNO (Associate Professor),
Asako MURATA (Assistant Professor)

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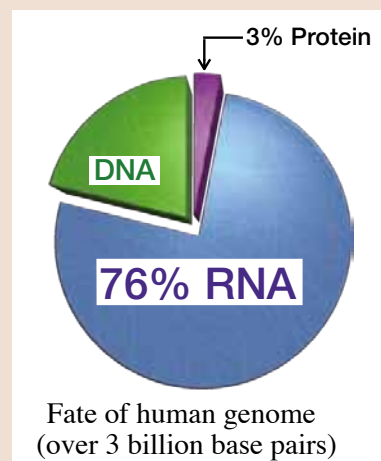
Home Page http://www.sanken.osaka-u.ac.jp/labs/rbc/english/index_e.html

[Research Interests]

- 1) Chemical Biology of trinucleotide repeats
- 2) Regulation of gene expression by synthetic small molecule
- 3) Development of small molecule targeting functional RNAs
- 4) Development of really useful method for genetic diagnosis

With the technique of accurate synthetic organic chemistry and the knowledge and sense for treating nucleic acids as organic molecules, we focused our research attention on small molecules targeting DNA and RNA that regulates biological functions. Most part of human genome (76%) is transcribed into RNA that does not encode any protein. These non-coding but functional RNAs are important targets for small molecules to regulate biological function. With these studies, we may achieve to develop new technology for human society and to open a new ear in genome science. Toward this end, we have set very challenging research

themes. Two approaches, one is from synthetic chemistry and the other is from molecular biology were effectively combined to launch creative studies on these projects.



Department
of
Chemistry

Laboratory for Synthetic Organic Chemistry

(The Institute of Scientific and Industrial Research)

Members Hiroaki SASAI (Professor), Shinobu TAKIZAWA (Associate Professor), Kazuhiro TAKENAKA (Assistant Professor), Makoto SAKO (Assistant Professor)

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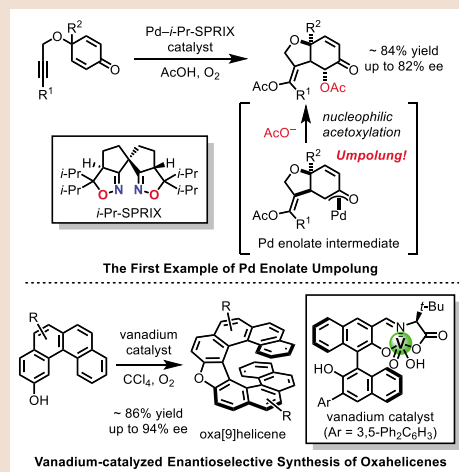
Home Page http://www.sanken.osaka-u.ac.jp/labs/soc/socmain_english.html

[Research Interests]

- 1) Efficient synthesis of advanced materials utilizing chiral spiro compounds
- 2) Establishment of practical enantioselective reactions based on a new concept
- 3) Development of multifunctional organocatalysts and their application to environmentally benign process
- 4) Development of green sustainable organic reactions using reusable solid-supported catalysts

The goal of this laboratory is to develop catalytic asymmetric processes that produce optically active organic compounds with high selectivity. We have already developed heterobimetallic complexes that promote a variety of asymmetric reactions in a manner analogous to enzymatic reactions. Now, we engage in the design and synthesis of novel optically active catalysts and reaction media based on a new concept, and their application to the energy-saving and environment-conscious reactions directed

towards practically useful processes. Theoretical studies on design of catalysts and reaction mechanism are also conducted.

Department
of
Chemistry

Laboratory of Protein Organic Chemistry

(Institute for Protein Research)

Members Hironobu HOJO (Professor), Toru KAWAKAMI (Associate Professor), Yuya ASAHINA (Assistant Professor)

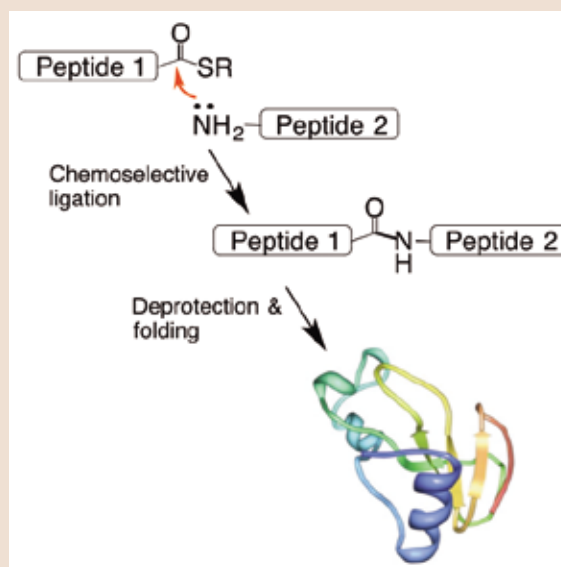
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[Research Interests]

- 1) General studies on a chemical protein synthesis
- 2) Development of methods for peptide ligation
- 3) Synthesis, structural and functional studies of membrane proteins
- 4) Synthetic studies of post-translationally modified proteins

Chemical methods enable the synthesis of proteins, which can not be prepared by the recombinant method, such as site-specifically labeled, glycosylated and phosphorylated proteins. Laboratory of Protein Organic Chemistry is aiming to promote new protein researches using these synthetic proteins. Thus, our laboratory is developing facile methods for protein synthesis based on ligation chemistries. In addition, the synthetic method is applied for the preparation of membrane proteins and their partial sequences to elucidate the signal transduction mechanism by solid state NMR and IR. Modified histones and their partial sequences, glycosylated proteins are also being synthesized for the functional analyses.



Department
of
Chemistry

Laboratory for Molecular Biophysics

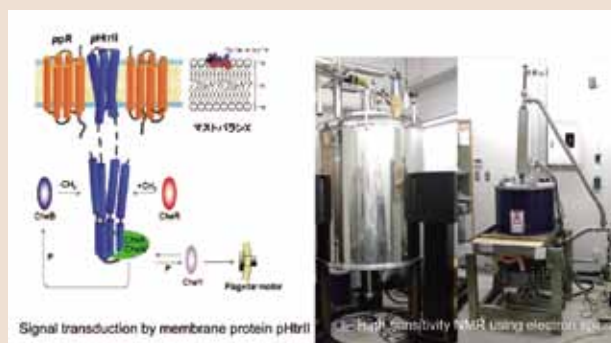
(Institute for Protein Research)

Members Toshimichi FUJIWARA (Professor), Yohei MIYANOIRI (Associate Professor, concurrent), Yoh MATSUKI (Assistant Professor)**Tel · Fax** Tel: +81-6-6879-8598 · Fax: +81-6-6879-8599 **e-mail** tfjwr@protein.osaka-u.ac.jp**Home Page** <http://www.protein.osaka-u.ac.jp/biophys/>**[Research Interests]**

- 1) Structure of membrane proteins pHtrII for transmitting light signal and halorhodopsin for light-driven ion pumping
- 2) Development of high-sensitivity NMR using hyperpolarization by terahertz wave irradiation
- 3) Structure analysis by NMR bioinformatics
- 4) Elucidation of the correlation between structure, dynamics and function of large molecular proteins using NMR

Solid-state NMR reveals structure and function of biologically important molecular complexes that are not amenable to X-ray crystallography and solution NMR. These systems include proteins tightly bound to lipid bilayers and noncrystalline large molecular complexes, such as membrane protein pHtrII for the transmission of light signal, halorhodopsin for light-driven ion pumping, transmembrane domains of proton ATP synthase, and model G-protein-receptor complexes. We are also developing NMR methods by using advanced technologies for NMR experiments,

bioinformatics and molecular biology. One of NMR spectrometers features high-power terahertz wave source, gyrotron, for enhancing the sensitivity by using electron spin polarization.

Department
of
Chemistry

Laboratory of Protein Profiling and Functional Proteomics

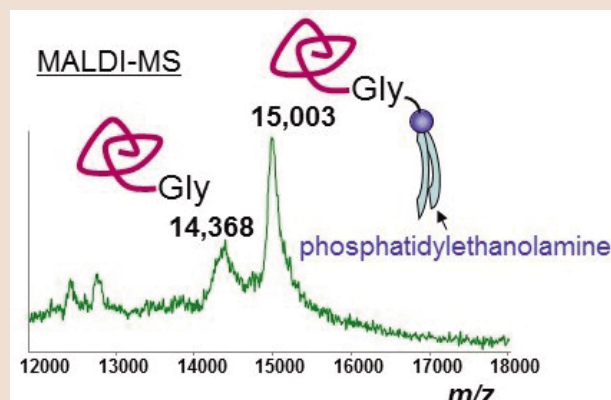
(Institute for Protein Research)

Members Toshifumi TAKAO (Professor)**[Research Programs]**

- 1) Development of chemical/analytical methods and soft-ware for analysis of protein primary structure.
- 2) Hardware development for high-sensitivity MS.
- 3) MS analysis of post-translational modifications.
- 4) Development of a chemical derivatization method for high sensitive detection of sugar chains.
- 5) Development of chemical and separation methods for proteomic analysis.
- 6) Study on fragmentation of peptides and carbohydrates in MS.

Mass spectrometry (MS) is a well accepted technique for the analyses of chemical structures of biological compounds. We have been working to develop methods for determining primary structures and post-translational modifications of proteins by using MS. In conjunction with accumulating protein and gene sequence databases, we are using state-of-the-art MS for large-scale protein identification which is indispensable for proteomics research. We also apply the above developed methods to the structural analysis

of micro quantities of peptides, proteins, and their related substances.



Department
of
Chemistry

National Institute of Advanced Industrial Science and Technology (AIST)

Inorganic Functional Materials Research Institute

Members Kenji KAMADA (Guest Professor)**Tel · Fax** Tel: +81-72-751-8609 · Fax: +81-72-751-9637 **e-mail** k.kamada@aist.go.jp**[Research Area]**

- 1) Structure-property relationship of two-photon absorption of π -conjugated molecules.
- 2) Multi-photon absorption materials, nonlinear refractive-index-change materials.
- 3) Measurement technology of nonlinear optical properties.

Two-photon absorption (2PA) is a phenomenon whereby two photons are simultaneously absorbed by a molecule. This process has been used for 3D-resolved fluorescence imaging of living tissues and now is expected as a key process for terabyte-class large-capacity optical memories. However, high-sensitive 2PA materials are needed for applications with less intense laser pulses because 2PA occurs under intense optical field. We focus our activities on clarifying the structure-property relationship, i.e. what kind of molecular structures give excellent 2PA sensitivity, by means of 2PA spectral measurements with femtosecond laser pulses and theoretical calculation of the electronic states based on the first principle. In addition, we develop and characterize novel multi-photon absorption materials and nonlinear refractive-index-change materials by worldwide collaborations. Moreover,

methodology for reliable, reproducible measurements of nonlinear optical properties is also an important subject. With these activities, we will create novel organic materials with high functionality for photonics and establish basic theoretical framework for the developments.

Department
of
Chemistry

National Institute of Advanced Industrial Science and Technology (AIST)

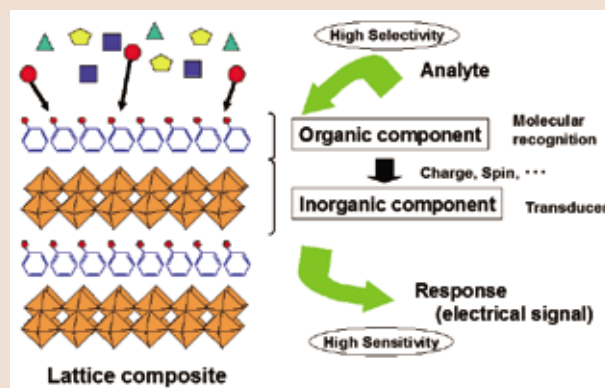
Inorganic Functional Materials Research Institute

Members Ichiro MATSUBARA (Guest Professor)**Tel · Fax** Tel: +81-72-751-8360 · Fax: +81-72-751-9970 **e-mail** matsubara-i@aist.go.jp**[Research Programs]**

- 1) Lattice composites
- 2) Organic-inorganic hybrid materials
- 3) Development of high performance gas sensors by novel materials
- 4) Preparation process of metal oxide nanoparticles

We have proposed the concept of 'lattice composite', and we are developing new gas sensing materials based on the concept. Crystal lattice is recognized as a smallest unit which can generate a function. The composites of different kind of lattices can be expected to generate a new function or an advanced function by synergetic effects of the lattices. In order to develop novel gas sensing materials, we have expanded the concept not only to inorganic compounds but also to organic compounds. Gas sensing materials have two elemental functions, molecule recognition and transducer. The shearing of the elemental functions by both the

components can realize high performance sensing properties in the lattice composite materials.



Department
of
Chemistry

National Institute of Advanced Industrial Science and Technology (AIST) Research Institute of Electrochemical Energy

Members Nobuhiro KURIYAMA (Guest Professor)**Tel · Fax** Tel: +81-72-751-9611 · Fax: +81-72-751-9629**e-mail** kuriyama-n@aist.go.jp**Home Page** http://unit.aist.go.jp/reiecen/index_en.html**[Research Interests]**

- 1) Batteries (Lithium-ion batteries, Ni-metal hydride batteries, etc.)
- 2) Fuel Cells (PEMFC, Direct fuel cells, etc.)
- 3) Chemical Energy (Hydrogen, Catalysts for environment, etc.)
- 4) Material Science (Microscopic analysis, First-principles calculation, "Materiomics", etc.)

The core of our research is surface science or interface science based mainly on electrochemistry and catalytic chemistry. The subject of this field is the phenomena that occur from interactions between solid substance and molecules such as reactions, permeation and absorption. These research works lead to storage and emission of chemical energy, which accompanies reversible transformations of materials, thereby making it indispensable basic technology for the technical deployment of compact and mobile

energy source and energy network. Most of them are interdisciplinary research projects collaborating with industry.

Department
of
Chemistry

Peptide Institute, Inc.

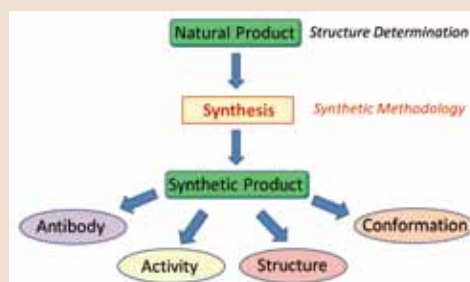
Members Hideki NISHIO (Guest Professor), Kumiko YOSHIKAWA-KUMAGAYE (Guest Professor), Toshihiro YAMAMOTO (Guest Associate Professor)**Tel · Fax** Tel: +81-72-643-4411 · Fax: +81-72-643-4422**Home Page** <http://www.peptide.co.jp/en>**e-mail** nishio@peptide.co.jp kumiko@peptide.co.jp yamamoto@peptide.co.jp**[Research Interests]**

- 1) Chemical Synthesis of Protein and Their Structure-Function Relationships.
- 2) Synthesis of Carbohydrate Conjugates and Evaluation of Their Functions.
- 3) Chemical Synthesis of Biologically Active Peptides and Elucidation of Their Structure-Activity Relationships.
- 4) Design and Chemical Synthesis of the Enzyme Substrates and Inhibitors.

Our laboratory has been mainly involved in the development of synthetic methodology of large peptides, proteins, and carbohydrate conjugates. For the synthesis of large peptides or proteins, we utilize the segment condensation method applying the maximum protection strategy in solution. The peptide segments can be synthesized by our solid phase synthetic strategy, and each segment is coupled in solution to obtain long protected peptides which are then treated with anhydrous hydrogen fluoride to obtain free peptides. In order to overcome the problems encountered during synthesis, we are developing protecting groups and/or solvent systems that are available to our synthetic strategy. For the multiple cysteine-containing peptides, the various disulfide bond

formations in one molecule are analyzed and the relationship between conformation and the ratio of disulfide isomers are investigated. For the synthesis of the carbohydrate conjugates, we are evaluating the stability of glycoside bonds in several kinds of sugar under the deprotecting conditions and developing synthetic strategy of carbohydrate moiety.

In order to elucidate the mechanism of biological phenomenon, we are always making efforts to supply reliable synthetic samples of peptides and carbohydrate conjugates for the collaboration with many researchers.



Department
of
Chemistry

Suntory Foundation for Life Sciences, Bioorganic Research Institute

Members Keiko SHIMAMOTO (professor)

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[Research Interests]

- 1) Function of Novel Glycolipids
- 2) Function of Lipids in Biomembranes
- 3) Chemical Syntheses of Bioactive Probes

Many biological events involve not only proteins but also non-proteinaceous molecules such as small bioactive compounds, carbohydrates, and lipids. In order to elucidate the mode of action, it is necessary to identify the involved molecules by means of advanced instrumental analysis such as NMR and MS, and to develop molecular probes chemically synthesized.

Biomembranes include small amounts of glycolipids as well as phospholipids, however, the roles of such minor components and their biological significance remain unsolved. The difficulty in molecular biological approach is one of the reasons for the delay of elucidation of biomembrane functions. By using techniques of organic chemistry, we identified the structure of a novel glycolipid,

MPIase, essential for the membrane protein integration. We study on the activity mechanisms of MPIase by chemically synthesizing molecular probes and by building simple model system for analyses of the interaction between membranes and the glycolipid.

