Department of Chemistry

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

Synthetic organic experiment using exhaust equipment for safety biomimetic model compound of the active site of metalloproteins, and the model complexes are structurally and functionally compared with the active site of proteins.

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.

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.

Interdisciplinary Chemistry Division

In this Division research works are oriented towards novel fields of both bioorganic and bioinorganic chemistry. 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. 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.

Home Page

http://www.chem.sci.osaka-u.ac.jp/graduate/chem-e/index.html

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 Biomolecular Chemistry
13. Laboratory for Organic Biochemistry

Interdisciplinary Chemistry Division

14. Laboratory for Natural Product 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. Laboratory for Isotope Chemistry, Institute for Radiation Sciences

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 Complex Molecular Chemistry
24. Laboratory for Synthetic Organic Chemistry

Institute for Protein Research (Cooperative Division)

25. Laboratory of Protein Organic Chemistry
26. Laboratory for Molecular Biophysics
27. Laboratory of Protein Profiling and Functional Proteomics
28. Laboratory for Computational Biology

Cooperative Adjunct Division

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

Department of Chemistry

Laboratory for Analytical Chemistry

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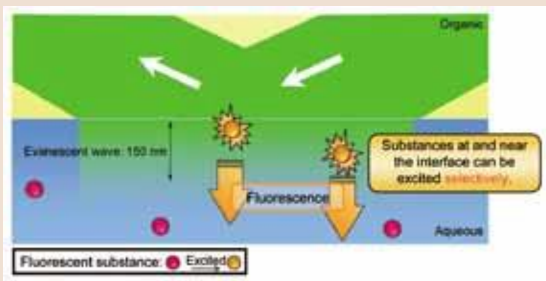
[Research Interests]

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.



Total internal reflection excitation method

Department of Chemistry

Laboratory for Radiochemistry

Members Atsushi SHINOHARA (Professor), Yoshitaka KASAMATSU (Associate Professor), Kazuhiko NINOMIYA (Assistant Professor)

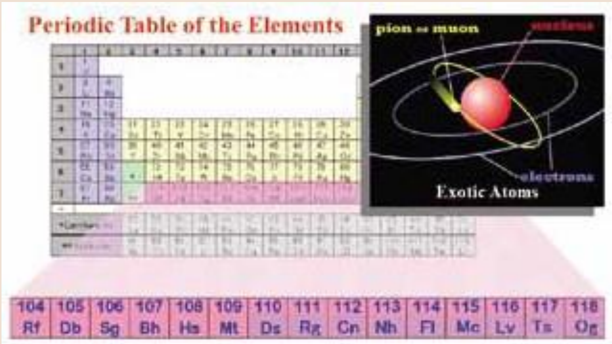
Home Page http://www.chem.sci.osaka-u.ac.jp/lab/shinohara/index_e.html

[Research Area]

1) Chemistry of superheavy elements
2) Chemistry of exotic atoms
3) Development of radionuclides for medical use (mainly on targeted alpha therapy)
4) Environmental radioactivity of Fukushima Nuclear accident origin
5) 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.



Department of Chemistry

Inorganic Chemistry Group

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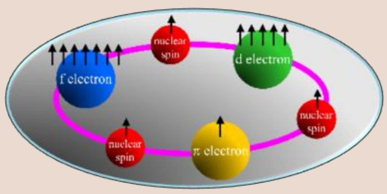
[Research Interests]

1) Electronic structure and molecular magnetism of the systems containing 4f electrons.
2) New molecular devises 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.



Department of Chemistry

Laboratory for Bioinorganic Chemistry

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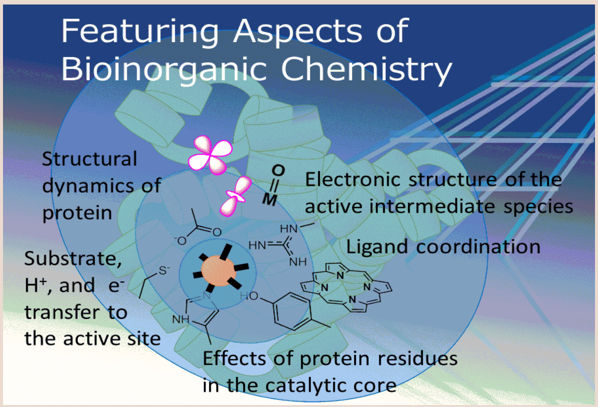
[**Research Interests**]

1) Synthesis of dinuclear and multinuclear metal complexes activating molecules
2) Synthesis of heterometallic multinuclear complexes activating molecules
3) Synthesis of novel metal complexes as a photosensitizer
4) Development of artificial metalloenzymes activating molecules
5) Investigation of relationships between structures and functions of metalloprotein
6) Synthetic and mechanistic study on metal complexes with anticancer activity

The photosynthetic energy transduction and metabolism involve photo-excitation coupled with electron transfer process, and activation of substrates including small molecules such as O_2 and N_2. The 1st transition metals are frequently essential trace elements for organisms, working at the active sites in the proteins. The metal complexes sometimes show pharmaceutical activity. We study on metals in biology, and we newly develop relevant metal complexes and metalloenzymes.



Department of Chemistry

Laboratory for Condensed Matter Physical Chemistry

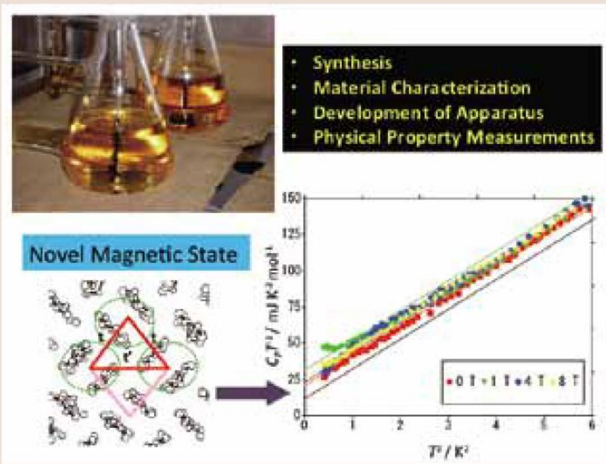
Members Yasuhiro NAKAZAWA (Professor), Hiroki AKUTSU (Associate Professor) Satoshi YAMASHITA (Assistant Professor)

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.



Department of Chemistry

Laboratory for Surface Chemistry

Members Hiroyuki S. KATO (Associate Professor), Takashi YAMADA (Assistant Professor)

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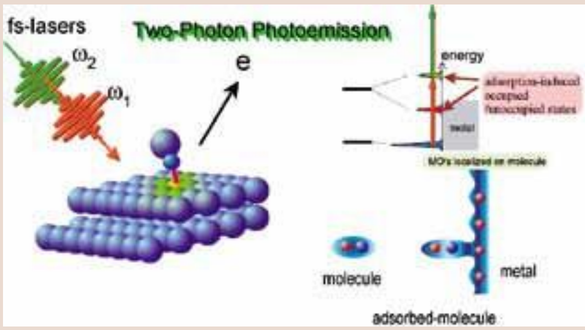
[Research Interests]

(1) Photoemission microspectroscopy 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 surface 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.

Department of Chemistry

Laboratory for Quantum Chemistry

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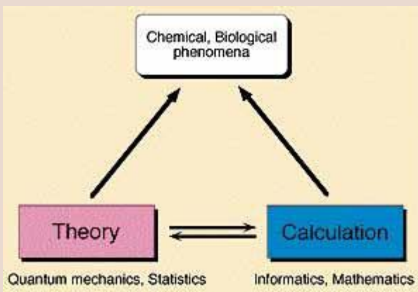
［Research area］

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 of 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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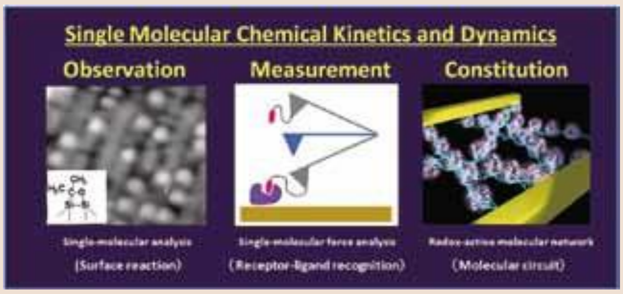
[Research Interests]

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.



Department of Chemistry

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.

Department of Chemistry

Laboratory for Beam Chemistry

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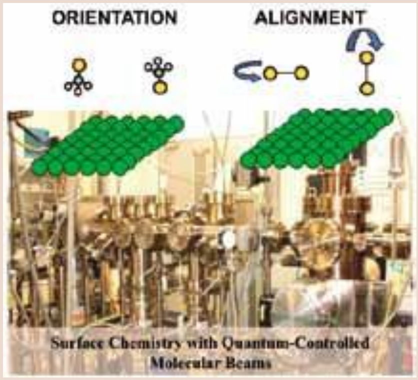
[Research Interests]

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

We mainly focus on surface chemistry explored with newly developed original experimental techniques and their related equipments.

Particularly, our 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.



Department of Chemistry

Laboratory for Structural Organic Chemistry

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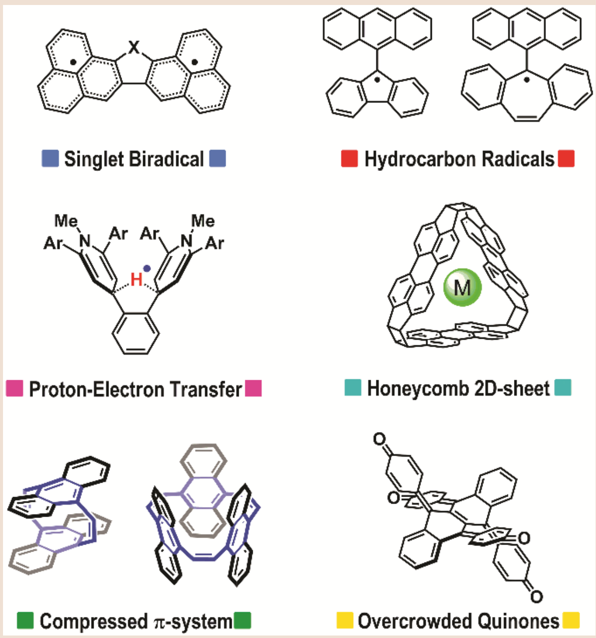
[Research Interests]

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, 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.



Department of Chemistry

Laboratory for Physical Organic Chemistry

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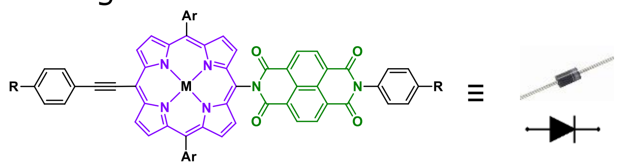
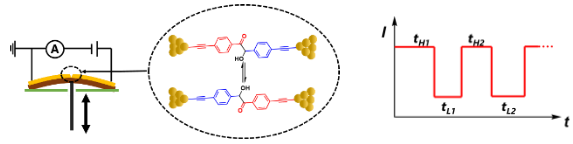
[Research Interests]

1. Single-molecule Science: molecular electronics & single-molecule chemical reaction
2. Development of novel application of antiaromatic molecules
3. Development of the new chemistry of stacked (anti)aromatic molecules.
4. Luminescent molecules: solid-state emission & mechanochromism

■ Single-molecule rectifier



■ Single-molecule chemical reactions



■ Single molecule magnets (SMMs)

Department of Chemistry

Laboratory for Biomolecular Chemistry

Members Michio MURATA (Professor), Shinya HANASHIMA (Associate Professor), Yuichi Umegawa (Assistant Professor)

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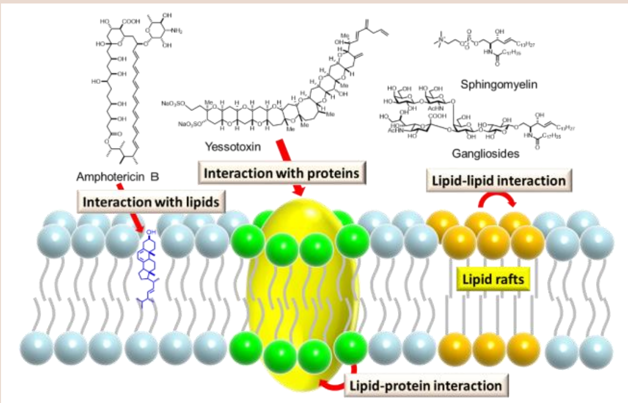
[Research Interests]

1. Action of drugs and natural products in biological membranes
2. Dynamic lipid conformations in bilayer membranes
3. Lipid-lipid and lipid-protein interaction at lipid rafts
4. Synthesis of complex natural products

We are interested in the membrane active drugs and toxins, as well as the endogenous lipids and sterols to elucidate the active molecular assemblages. Chemical synthesis assisted NMR analysis works out the channel structure of the polyene antibiotics-lipids assembly, dynamic lipid conformations and lipid interactions occurring in bilayer membrane.



Department of Chemistry

Laboratory for Organic Biochemistry

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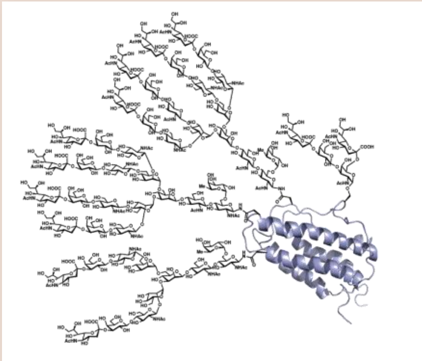
[Research Interests]

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). We have also evaluated the effect of oligosaccharide during protein folding process.



Department of Chemistry

Laboratory for Natural Product Chemistry Group

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Atsushi SHIMOYAMA (Assistant Professor), Yoshiyuki MANABE (Assistant Professor)

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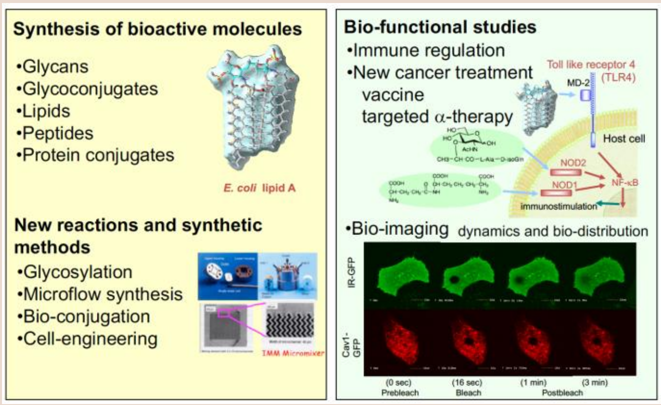
［Research Interests］

- Chemistry and function of immunomodulating substances from microbes and hosts
- Efficient and selective methods for glycosylation and oligosaccharide synthesis
- Bio-imaging of glycans and proteins for the new functional studies
- Targeted α-radiation therapy for cancer

We have studied the syntheses and biofunctions of microbial and host-derived molecules related to important biological phenomena such as immunity, infection, allergy, cancer, and etc. In particular, we have investigated glycans and glyco-conjugates in order to identify the active principle, elucidate the action mechanism, and control the biological responses. Bio-imaging study of glycans, peptides, and proteins have been investigated by using fluorescent microscopy. Targeted α-particle therapy for cancer is also important project.



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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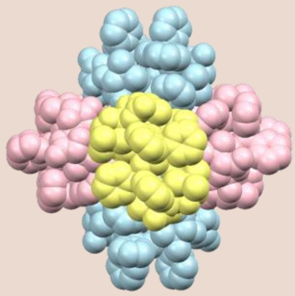
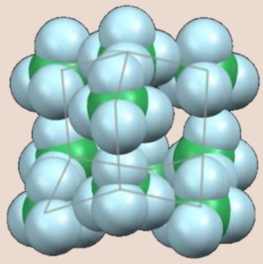
[Research Interests]

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. Our current interest is directed toward the development of fundamental coordination chemistry by utilizing multifunctional metalloligands by using simple ligands.





Department of Chemistry

Research Center for Thermal and Entropic Science

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

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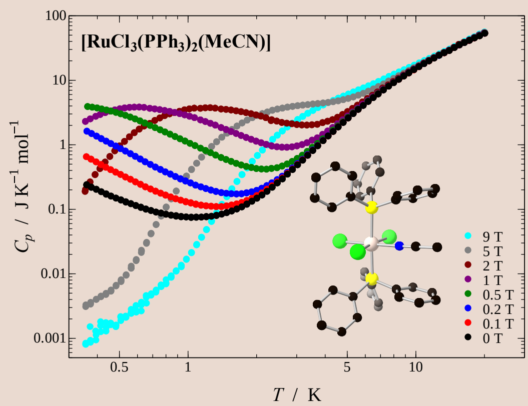
[Research Interests]

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.



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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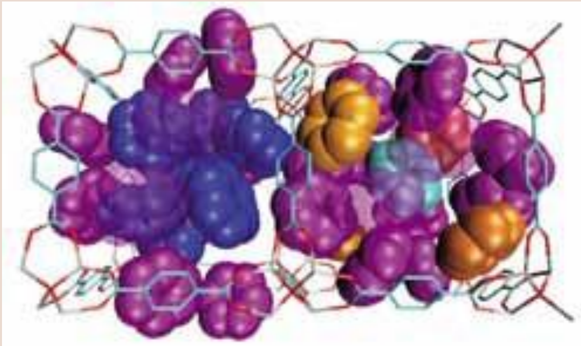
Home Page https://chemistry.museum.osaka-u.ac.jp/chemistry/research-en/

[Research Interests]

1) Construction of new molecular assembly using a uniquely restricted nanospace and investigation of their novel properties
2) Development of new porosimetry based on NMR spectroscopy

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



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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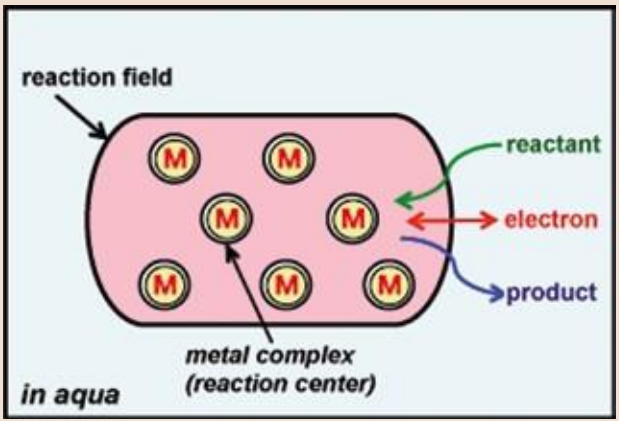
[Research Interests]

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 filed 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

Laboratory for Isotope Chemistry

(Institute for Radiation Sciences)

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

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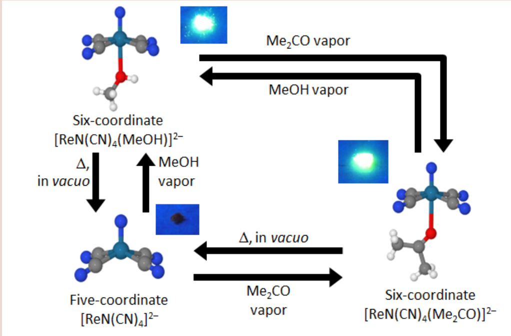
［**Research Interests**］

1) Synthesis of new chelate agents for nuclear medicine
2) Synthesis and photoluminescent properties of metal complexes
3) Synthesis and properties of actinide complexes
4) Development of agents for separation of lanthanides and actinides

Radioactive elements account for nearly one third 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 chelating agent for nuclear medicine. We are interested in synthesis of new photoluminescent metal 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.



Department of Chemistry

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

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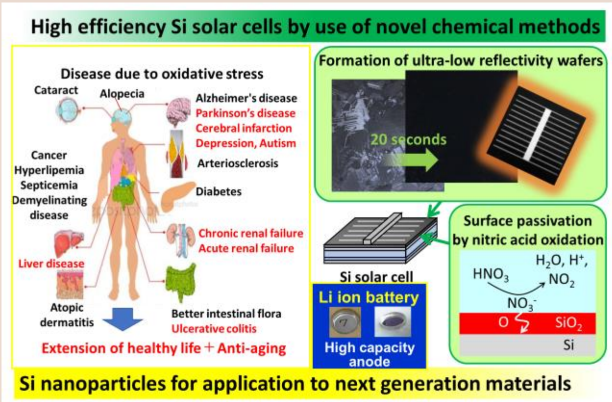
［Research Interests］

1) High efficiency Si solar cells by use of new chemical methods.
2) Si nanoparticles for application to next generation materials.

Conversion efficiencies of Si solar cells are much lower than theoretical limit of ~30%. New chemical methods to prevent reflection at Si surfaces and recombination of electrons and holes have been developed to improve the efficiency of Si solar cells.

We have developed Si-based agent which can continuously generate a high amount of hydrogen in bowels. Si-based agent has been found to be effective to prevent various oxidative stress-induced diseases such as chronic renal failure and Parkinson's disease.

High capacity anodes for lithium ion batteries have also been developed using silicon swarf (industrial waste) generated with a high amount during production of Si wafers for solar cell use.



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.

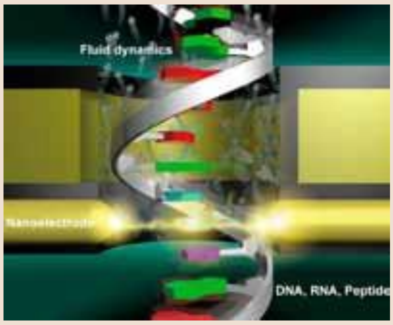

Fig. Shematic of single-molecule sequencing method.

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 (Associate Professor), Tomonori SHIBATA (Assistant Professor), Takeshi YAMADA (Assistant Professor)

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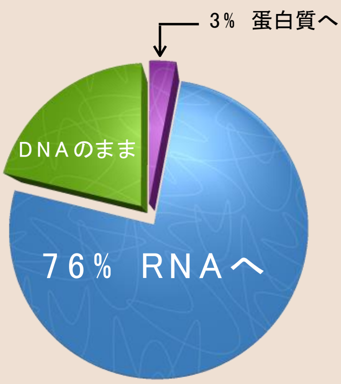
[Research Interests]

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.



ヒトゲノム30億塩基対の使われ方

Department of Chemistry

Laboratory for Complex Molecular Chemistry

(The Institute of Scientific and Industrial Research)

Members Takayoshi SUZUKI (Professor), Yasunobu YAMASHITA (Assistant Professor)

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[Research Interests]

1) Development of epigenetic inhibitors and their applications
2) Target-guided synthesis of enzyme inhibitors
3) Chemical biology and medicinal chemistry for refractory diseases
4) Medicinal chemistry using artificial intelligence

Aiming to develop therapeutic agents and chemical probes, medicinal chemistry and chemical biology studies are conducted in our group. The focused fields of computational molecular design, synthetic reactions, and biological action mechanisms of bio-functional molecules are studied on the basis of organic chemistry. For example, we are working on the development of epigenetic inhibitors and their applications. Epigenetic mechanisms including DNA methylation and histone modifications are regulated by enzymes. The epigenetic proteins form complexes by protein-protein interactions and protein-lncRNA interactions, which regulates epigenetic gene expression. We are trying to identify small molecules that inhibit the function of the complexes and to apply the small molecules to chemical biology studies and drug discovery.

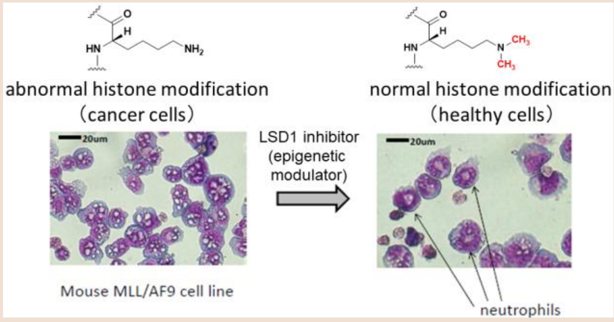

Fig. Cancer therapy by epigenetic modulators.

Department of Chemistry

Laboratory for Synthetic Organic Chemistry

(The Institute of Scientific and Industrial Research)

Members Hiroaki SASAI (Professor), Shinobu TAKIZAWA (Associate Professor), Masaru Kondo (Assistant Professor)

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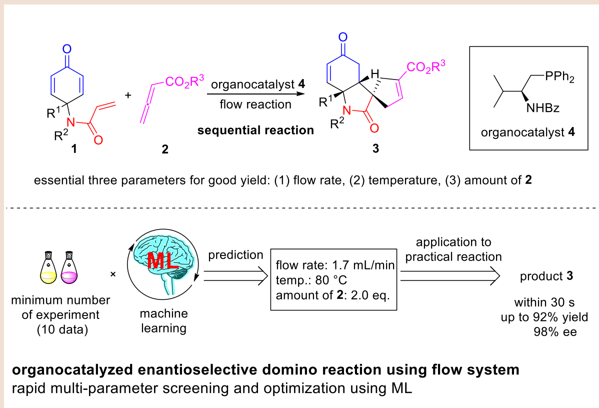
[Research Interests]

1) Establishment of practical enantioselective reactions based on a new concept
2) Development of multifunctional organocatalysts and their application to environmentally benign process
3) Development of efficient parameter screening and optimization methodology using machine learning

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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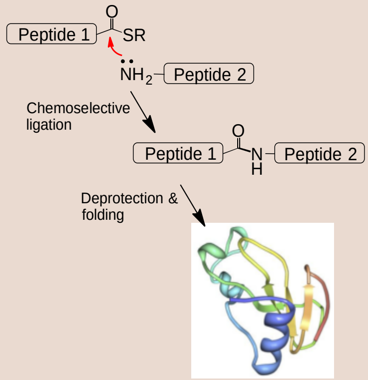
［Research Interests］

1. General studies on a chemical protein synthesis
2. Development of methods for 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 synthesisof 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.



General procedure for chemical protein synthesis.

Department of Chemistry

Laboratory for Molecular Biophysics

(Institute for Protein Research)

Members Toshimichi FUJIWARA (Professor), Yoh MATSUKI (Associate Professor), Yohei MIYANOIRI (Associate Professor, concurrent)

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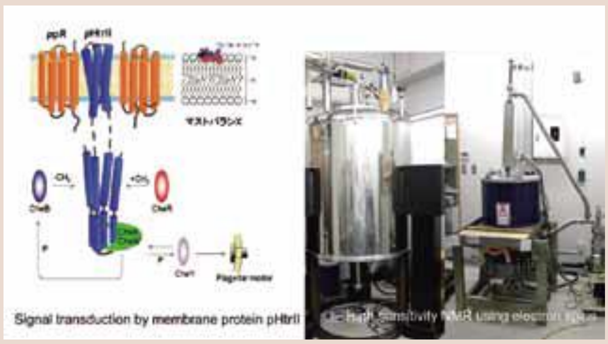
Home Page http://www.protein.osaka-u.ac.jp/biophys/

［Research Interests］

1) Structure of membrane proteins *p*HtrII 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

NMR reveals structure and function of biologically important molecular complexes that not amenable to X-ray crystallography and electron microscopy. These systems include proteins 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, amyloid protein fibers, and model G-protein-receptor complexes.

We are also developing NMR methods by using advanced technologies for NMR experiments, bioinformatics and molecular biology. Two NMR spectrometers features high-power terahertz wave sources, 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), Toshiki TAKEI (Assistant Professor), Qiuyi WANG (Specially Appointed Assistant Professor)

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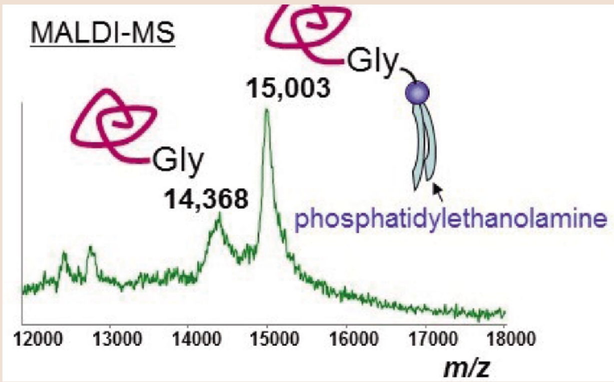
[Research Programs]

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

Laboratory for Computational Biology
(Institute for Protein Research)

Members Kenji MIZUGUCHI (Professor), Chioko NAGAO (Assistant Professor)

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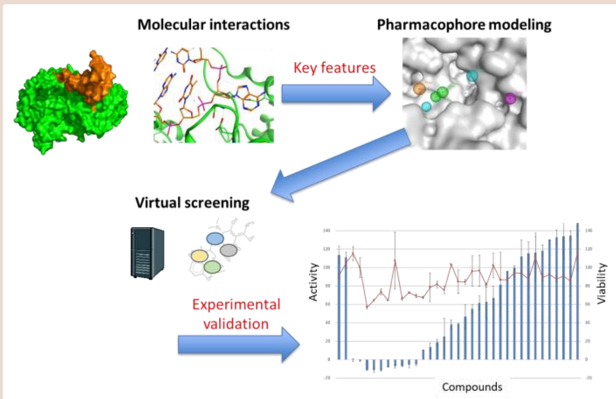
Home Page https://mizuguchilab.org/

[Research Interests]

1) Data integration for relating molecular-level events with higher-order biological systems.
2) Understanding and predicting molecular interactions involving proteins, and modelling biological responses

We aim to increase our understanding of biological systems and diseases by combining computer science and computational chemistry approaches, with applications to drug discovery and other research areas. Artificial Intelligence (AI) is expected to play major roles in many domains. Recognizing that the availability of a large amount of data in a computer-friendly format is key to the successful development of AI models, our research is focused on integrating a wide array of data, including genes, proteins, chemical compounds and diseases. We also develop methods for predicting protein structure, function and interaction, and apply them to real-life data analysis.



Department of Chemistry

National Institute of Advanced Industrial Science and Technology (AIST), Kansai Center
Nanomaterials Research Institute (NMRI)

Members Kenji Kamada
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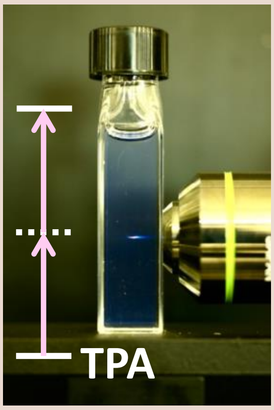
［Research Topics］

1) Highly-sensitive TPA materials and their structure-property relationship.
2) Photon upconversion materials operating at the sunlight-level intensity and triplet exciton dynamics, especially in solid.

We are working in a new field, so-called 'Two-Photon Photochemistry' which will open new functionalities of materials by two photons but cannot be achieved by one photon. One of such topics is **Two-Photon Absorption (TPA)** and another is **Photon Upconversion** via triplet excited state, allowing a new way to use photon energy efficiently.



Spatial selective photo-excitation by two-photon absorption (above).

Crystalline solid showing blue emission by green excitation at sunlight level, (from long to short wave-length conversion, below).

Department of Chemistry

National Institute of Advanced Industrial Science and Technology (AIST)
Innovative Functional Materials Research Institute

Members Ichiro MATSUBARA (Guest Professor)
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Home Page https://unit.aist.go.jp/ifm-ri/index_en.html

［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.

Gas sensing materials have two elemental functions, molecule recognition and transducer. The shearing of the functions by both the components can realize high performance sensing properties.

Department of Chemistry

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

Members Nobuhiro KURIYAMA (Guest Professor)

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[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 YOSHIZAWA-KUMAGAYE (Guest Professor), Toshihiro YAMAMOTO (Guest Professor)

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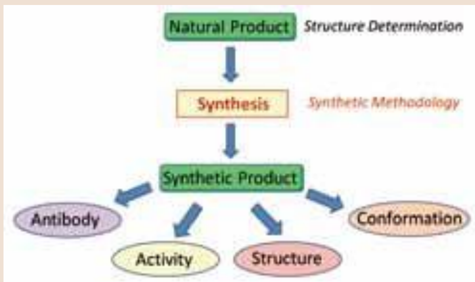
[Research Interests]

1) Chemical Synthesis of Protein and Their Structure-Function Relationships.
2) Synthesis of Carbohdrate 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 cystine-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.