

# Laboratory Guide

School of Materials Science

Japan Advanced Institute of Science and Technology

### FUJIMOTO Lab.

### Professor : FUJIMOTO Kenzo E-mail : kenzo@jaist.ac.jp

[Research areas] Nucleic acids chemistry, chemical biology [Keywords] Nucleic acid drug. Photochemical genome editing. organic synthesis, genetic diagnosis

# Development of nucleic acids drug based on creation of designed molecules



### Skills and background we are looking for in prospective students

In our laboratory, "Understanding the fundamental principles of science, by creating and designed original molecules combined with a rational and precise approach having special physical properties" is the main challenge. We develop new methods to further challenge various domains of science and welcome people with creative ideas to tackle these challenges from different scientific backgrounds.

### What you can expect to learn in this laboratory

In this laboratory, we try to understand and develop natural/biological phenomena through the study of journal papers, study groups, scientific experimentations, research presentations, and other unique and innovative approaches. Initiatives taken to support students to grow their intellectual toughness:

- Laboratory seminar by eminent professors working in the major fields of science Participation in technical schools held in Tokyo and Osaka Academic conferences (domestic and international)
- Support for publishing in international scientific journals
- Active participation in venture laboratories
- Joint seminar and exchange with collaborative research companies

[Job category of graduates] Employment opportunities: University faculty, chemical industry, pharmaceutical companies, mechanical companies, electrical companies, research scientist, medical equipment companies, food industry etc.

### **Research outline**

Modern genetic engineering technology is currently based on enzymes for the in vivo genetic manipulations. Moreover, the micro-robotics is also limited by the enzymes. In Fujimoto Lab, we use photo-responsive artificial nucleic acid to tackle the problem of genetic engineering with high specificity and precision through organic chemical approach coupled with photo-chemistry. We have developed a novel approach to manipulate the DNA or RNA using light instead of enzymes.

This research falls under inter-disciplinary research combining molecular biology, organic chemistry, information science, cell biology, and other fields. We are developing a strong and industrially viable approach for applications such as gene manipulation and analysis.

Upon UV radiation, DNA can get damaged by the formation of a pyrimidine dimer in the DNA strand. This [2+2] photo-cyclization reaction can be exploited using a photo-active vinyl group. To manipulate the nucleic acid using light, we require an artificial photo-reactive nucleobase incorporated in the DNA strand using synthetic organic chemical methods.

In our lab, we synthesize these photo-active DNA probes and incorporate them into the DNA strand to accomplish the branching of DNA which is otherwise not possible in the naturally occurring DNA strands. We have successfully created a complex DNA origami structure using the photo-chemical approach. Also, we can utilize this photo-chemical approach in the DNA chip to analyze human genome at the single base level with an accuracy 100 times higher than the conventional methods.

These phenomena are successful due to a particular artificial photo-active nucleobase called cyanovinylcarbazole (cnvK) which can cross-link to nucleic acid in a matter of few seconds upon light radiation. Using cnvK, ultrafast plasmid manipulation, cytosine to uracil conversion, gene repair, and genetic engineering has been achieved. It is also expected to be utilized for the ultrafast genetic analysis on a microchip for future medical technology applications.

Focusing on the programmability of DNA molecules, basic elements (AND, OR, NOT, etc.) can be implemented using DNA nanotechnology. To further realize advanced information processing, the calculation mechanism (status transition) for determining the next output based on the past inputs and the current input in the cellular machine it is essential to realize the chemical reaction in vitro to calibrate the circuit.

There has been no study on these kinds of circuits in the literature. In Fujimoto laboratory, the original [2 + 2] DNA photo-ligation reaction through photo cyclization reaction binds two DNA molecules using a template DNA and utilize the fact that this system use simple basic reaction elements (AND, OR, NOT, etc.) to successfully organize and construct a full adder circuit for calculation of binary digits through DNA molecules. These outcomes beautifully integrate the biochemistry with information technology to further lead to the development of DNA molecular robots. This has been highly appreciated as the fundamental research to create a backbone for further interdisciplinary research areas such as molecular robotics.

### Key publications

- 1. T. Sakamoto, Z. Qiu, M. Inagaki. K, Fujimoto, Simultaneous amino acid analysis based on 19F NMR using modified OPA-derivatization method, Anal. Chem., 92, 1669-1673 (2020)
- 2. K. Fujimoto, H. Yang, S. Nakamura, Strong inhibitory effects of anti-sense probes on gene expression through ultrafast RNA photo-cross-linking, Chem. Asian. J., 14, 1912-1916 (2019)
- 3. K. Fujimoto, S. Sasago, J. Mihara, DNA photo-cross-linking using pyranocarbazole and visible light, Org. Lett., 20, 2802-2805 (2018)

### Equipment

Automatic DNA/RNA synthesizer, Laser confocal microscope, HPLC/UPLC, Microplate reader, Fluorescence spectrophotometer, UV-LED, Atomic force microscopy, Biacore, etc

### **Teaching policy**

#### [Website] URL: https://www.jaist.ac.jp/ms/labs/fujimoto/fujimotohp/

The fundamental of our research lies in the precise molecular design related to DNA and the rational organic synthesis technique based on it. As each student tackles the original research theme, we cultivate fundamental synthesis technology, analytical technology and scientific viewpoint to capture the essence of research. On top of that, the students experience collaborative research with chemical companies, medical device manufacturers and pharmaceutical companies and let them acknowledge researchers' ways to contribute to society. In addition, we aim to cultivate autonomous researchers by utilizing laboratory-specific programs (laboratory seminars, joint seminars, technical schools, etc.)

GOTOH Lab.

Professor : GOTOH Kazuma <sup>E-mail :</sup> kgotoh@jaist.ac.jp

[Research areas] Physical chemistry, Inorganic material chemistry [Keywords] Nuclear magnetic resonance, Carbon materials, Lithium ion batteries, Sodium ion batteries, in situ, operando analysis

# Nanospace Chemistry

## - Development of observation technology and controlling nanostructure -

### Skills and background we are looking for in prospective students

Basic knowledge of physical chemistry and inorganic chemistry is preferred. Motivation for learning basic skills and exploring novel phenomenon is required.

### What you can expect to learn in this laboratory

You will be engaged in experiments of material preparation, measurements using analytical equipment, and discussion about the experimentally obtained results. Thereby, you will learn skills about synthesis of inorganic materials, testing batteries, and analyses of materials using analytical methods such as solid state nuclear magnetic resonance (SSNMR). Furthermore, students will be trained through discussion to make great insights necessary to understand scientific phenomena: this capability for insight is most important for researchers and engineers.

[Job category of graduates] Researcher and engineer in manufacturing (chemistry, material, automobile, battery) or at research institutes

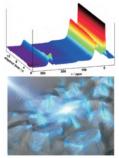
### **Research outline**

Our group emphasizes understanding of microscopic and mesoscopic structures and circumstances in nanospace of porous and layered materials such as carbon and inorganic compounds. The states and behaviors of molecules and ions in the nanospace are investigated using several analytical methods, especially solid state nuclear magnetic resonance (SSNMR). Because understanding of these technologies is essential for revealing the mechanisms of devices using the materials such as secondary batteries, we prospectively apply our technology to the development of such materials.

### "Reaction mechanism of lithium and sodium in electrode materials for next generation secondary batteries"

Lithium ion batteries (LIBs) are commonly used as indispensable energy storage systems for consumer electronics and vehicles. Sodium insertion materials have also attracted much attention for use in sodium ion batteries (NIBs), which are anticipated as a favorable alternative to LIBs because of their abundant resources and comparable electrode potential to that of LIBs. For LIB and

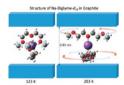
NIB development, elucidating the states of the lithium and sodium ions and the charging–discharging mechanism of the electrodes is indispensable. We are investigating the states of lithium and sodium in several electrode materials such as hard carbon, phosphorous, and layered 2D materials using <sup>7</sup>Li and <sup>23</sup>Na SSNMR (including *in situ* and *operando* measurements) to develop next-generation secondary batteries. Our research is aimed at developing methods to analyze the structures of electrodes and



alyze the structures of electrodes and the states of lithium and sodium in batteries, and to reveal lithium and sodium reaction mechanisms in electrode materials.

"Intercalation chemistry of inorganic layered compounds" Inorganic layered materials such as graphite intercalated compounds (GICs) are anticipated for several applications such as electrochemical devices, catalysts, superconducting materials, and precursors of thin film materials. We are studying the syntheses and properties of new GICs and layered materials intercalating alkali metal cations (Li<sup>+</sup>, Na<sup>+</sup>, or K<sup>+</sup>) and several organic molecules, which are anticipated for use as electrode materials or catalysts.

The structures and dynamics of intercalant molecules are investigated using X-ray diffraction and SSNMR to elucidate the interaction between intercalants and host materials. These analyses are crucially important for understanding the intercalation chemistry of new materials and the diffusion properties of alkali metals in 2D layers.



Reprinted from K.Gotoh et al., J. Phys. Chem C (2016).

### Key publications

- K. Gotoh\*, T. Yamakami, I. Nishimura, H. Kometani, H. Ando, K. Hashi, T. Shimizu and H. Ishida, Mechanisms for overcharging of carbon electrodes in lithium-ion/sodium-ion batteries analysed by *operando* solid-state NMR. *J. Mater. Chem. A* 8, 14472 (2020).
- R. Morita, K. Gotoh\*, K. Kubota, S. Komaba, K. Hashi, T. Shimizu and H. Ishida, Correlation of carbonization condition with metallic property of sodium clusters formed in hard carbon studied using <sup>23</sup>Na nuclear magnetic resonance. *Carbon* **145**, 712 (2019).
- R. Morita, K. Gotoh\*, M. Fukunishi, K. Kubota, S. Komaba, T. Yumura, N. Nishimura, K. Deguchi, S. Ohki, T. Shimizu and H. Ishida, Combination of solid state NMR and DFT calculation to elucidate the state of sodium in hard carbon electrodes. *J. Mater. Chem. A* 4, 13183 (2016).

### Equipment

Bruker AVANCE III 500 MHz-NMR (with SSNMR system containing *in situ* equipment)

X-ray diffractometer, X-ray photoelectron spectroscope, Thermal analyzer, Electron microscope, Gas adsorption analyzer, Electrochemical measurement devices, Cell assembly equipment (glovebox, etc.)

### **Teaching policy**

[Website] URL: https://www.jaist.ac.jp/nmcenter/labs/gotoh-www/home-en

I hope students will acquire both fundamental background as members of society and high expertise as specialists of physical and inorganic chemistry.

Seminars and group meetings in laboratories are held regularly. Each student should make a plan and have a schedule of their own experiments. Participating in collaborative research with other groups or companies is preferred for obtaining a wide scope for research.



# HO Lab.

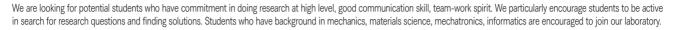
Professor: HO Anh Van

E-mail : van-ho@jaist.ac.jp

[Research areas] Intelligent robotics [Keywords] soft robotics, soft robotic hands, soft sensor, morphological computation, bio-inspired robots

# Utilization of materials softness in development of novel robotic mechanisms





### What you can expect to learn in this laboratory

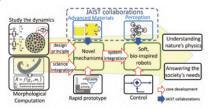
In our lab, we focus on new know-hows on development of soft robotic mechanisms, such as soft sensors, soft robotic hands, bio-inspired mechanisms. Students will have chance to learn how to design mechatronic systems using soft, flexible materials for specific applications that common rigid mechanisms cannot implement.

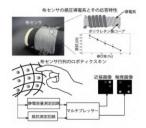
[Job category of graduates] Graduate students in lab are expected to design novel mechanisms, modelling physical phenomenon, conducting experiments, data analysis, and writing papers

### **Research outline**

Our Laboratory aims to answer emerging needs of the society by proposals of novel robotic systems, ranging from fabrication of sensors, actuators, and intelligence. We particularly focus on dynamic investigation of nature phenomena to find out the underlying, dominating mechanisms that could then give hints to fabrication of novel structures.

Ideas are shaped under the light of novel technologies with integration of scientific methods, then integrated in robotic systems with specific applications. Results obtained in this process could be inversely utilized to understand the natures.





### 1) Fabric Sensor with Proximity and Tactile Sensing:

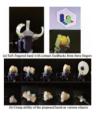
Human-in-the-loop task involving soft contact has become common in robotic application, especially in physical human-robot interaction. We attempt to fabricate a soft interface (or a robotic skin system) completely constructed from fab-

rics and soft materials that can sense both proximity and applied force from human's touch.

### 2) Soft robotic hand:

We proposed a novel approach to the fabrication of a soft robot-

ic gripper/hand with contact feedback for grasping delicate objects. Each finger has a multilayered structure, consisting of a main structure and sensing elements. The gripping energy of the fingers is generated from the elastic energy of the pre-stretched softer layers, and controlled by simple tendon strings pulled/released by a single actuation.



In addition, the hand includes a soft sensing elements for the detection of contact states with objects.

### 3) Bio-inspired mechanisms:

Nature is a great source of hints for development of bio-inspired robots. For example, we studied underlying physics of the wet adhesion mechanism of tree-frog's toes, and created a micro-structured soft pad for enhancement of contact force with adhesion in wet environment.

### **Key publications**

- J. Bernth, Van Anh Ho & Hongbin Liu, Morphological computation in haptic sensation and interaction: from nature to robotics, Advanced Robotics, Vol. 32, Issue 7, pp. 340-362, 2018
- Van Anh Ho et al., Wrin'Tac: Tactile Sensing System with Wrinkle's Morphological Change, IEEE Transactions on Industrial Informatics, Vol. 13, Issue 5, pp. 2496-2506, 2017
- Van Anh Ho and Shinichi Hirai, Design and Analysis of a Soft-Fingered Hand with Contact Feedback, IEEE Robotics and Automation Letters (RA-L), Vol 2, Issue 2, pp. 491-498, April, 2017.

### Equipment

3D- printer, NC machine, 6-dof industrial robot arm, milling cutter machine, 6-dof force/torque sensor, vacuum chamber

### **Teaching policy**

#### [Website] URL: https://www.jaist.ac.jp/ms/labs/vanho/index-e.html

Students will independently conduct research in collaboration with other members in the laboratory. Seminar is taken place one time a week, but meeting with supervisor can be setup any time upon demand. The supervisor will strictly follow the student's progress in research, and students must follow the PDCA (Plan-Do-Check-Action) cycle in research implementation. The supervisor will help students select suitable career path.

### HOHSAKA Lab.

Professor : HOHSAKA Takahiro <sup>E-mail :</sup> hohsaka@jaist.ac.jp

[Research areas] Genetic engineering, Protein chemistry [Keywords] Genetic code expansion, Nonnatural amino acid, Artificial protein, Cell-free translation, Fluorescence analysis

# Synthesis of artificial proteins by combining biological and chemical techniques



### Skills and background we are looking for in prospective students

Students should be interested in proteins and genes. Basic knowledge and experimental skills on biological chemistry and organic chemistry are required, but students will learn them after entering JAIST.

### What you can expect to learn in this laboratory

Students can learn professional knowledge and experimental techniques on genetic engineering, protein synthesis, organic synthesis, fluorescence analysis, etc. Through research activities, students can learn a series of research processes ranging from planning of experiments, investigation of related researches, acquisition and analysis of experimental data, summary of research results, and presentation of achievements. These abilities are indispensable as both researchers and engineers.

[Job category of graduates] Chemical or biological companies, research institutes

### **Research outline**

Our aim is to create new artificial proteins by combining biochemical techniques such as genetic engineering and protein synthesis with chemical methods such as organic synthesis. Specifically, we are pursuing the following research themes. We are also conducting research to make practical use of our achievements with companies.

### 1. Introduction of nonnatural amino acids into proteins by expansion of the genetic code

Proteins are made from amino acids according to the genetic code of DNA and show various biological functions by forming three-dimensional structures. However, only 20 types of amino acids are used in nature for protein biosynthesis. Beyond this limitation, we have succeeded in developing a new technology that can introduce artificially synthesized nonnatural amino acids into specific positions of proteins in response to expanded genetic code such as four-base codons (Fig.1).

### 2. Design and synthesis of artificial proteins

By using the above technology, we are working on design and function of artificial proteins with new functions. For example, protein sensors that can detect target molecules by fluorescence have been generated by introducing fluorescent nonnatural amino acids into ligand-binding proteins and antibodies (Fig.2). We are also tried synthesizing new protein or peptide drugs by utilizing the nonnatural amino acid incorporation technique. Parts of these studies are being in progress through collaboration with companies.

### Development of new biotechnologies using potential of organisms

It can be said that the nonnatural amino acid incorporation technique is derived from the potential function of organisms. We are trying to develop another biotechnology that can synthesize useful artificial proteins by utilizing new potential of organisms.

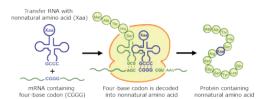


Fig. 1 Incorporation of nonnatural amino acids into proteins by using four-base codon.

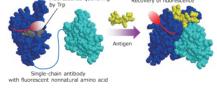


Fig. 2 Antibody-based fluorescence sensor.

### **Key publications**

- Double-fluorescent-labeled single-chain antibodies showing antigen-dependent fluorescence ratio change, K. Yoshikoshi, T. Watanabe, T. Hohsaka, *Bull. Chem. Soc. Jpn.*, 2016, 89, 573-580.
- Antibody-based fluorescent and fluorescent ratiometric indicators for detection of phosphotyrosine, K. P. Huynh Nhat, T. Watanabe, K. Yoshikoshi, T. Hohsaka, J. Biosci. Bioeng., 2016, 122, 146-154.
- "Quenchbodies": Quench-based antibody probes that show antigen-dependent fluorescence. R. Abe, H. Ohashi, I. Iijima, M. Ihara, H. Takagi, T. Hohsaka, H. Ueda, *J. Am. Chem.* Soc., 2011, 133, 17386-17394.

### Equipment

DNA analysis (DNA sequencer, real-time PCR, etc.), Fluorescence analysis (Fluorescence spectrometer, Fluorescence scanner, Fluorescence microscope, etc.), Mass spectrometer, Analytical and preparative HPLCs, etc.

### **Teaching policy**

#### [Website] URL: https://www.jaist.ac.jp/ms/labs/hohsaka/

Our goal is not only to obtain new knowledge from experiments but also to learn research process for artificial proteins. Specifically, we will train the ability to perform research such as planning the experiment, interpreting the result, solving the problem, feedback to the next experimental plan, etc. through repeated trial and error experiments. We regularly have research meetings for checking research status and providing guidance. We also have the opportunity to present the research results at academic conferences.

### KURISAWA Lab.

Professor: KURISAWA Motoichi <sup>E-mail :</sup> kurisawa@jaist.ac.jp

[Research areas] Biomaterials, drug delivery systems (DDS), nanomedicine, regenerative medicine [Keywords] Biodegradable polymers, nanoparticles, green tea catechin, injectable gel system, sustained drug release, drug targeting, cell therapy

# Enhancing Healing Power with Functional Biomaterials



### Skills and background we are looking for in prospective students

If you have basic knowledge of polymer chemistry, you can start your research without any problems. Still, we will give you profound guidance to play an active role in my laboratory, even if you do not have special knowledge and abilities before enrollment. In short, you can grow as much as you want, depending on your attitude toward daily research activities. To that end, I think it is crucial to create a laboratory where the spirit of mutual prosperity can be shared with research staff and students.

### What you can expect to learn in this laboratory

We design, synthesize, and characterize nanoparticles and gels and evaluate whether or not the desired function is sufficient through cell experiments and animal studies. By studying a wide range of fields, you will acquire the basics of various equipments and experimental methods. By the time you complete an animal experiment, you will develop the ability to make detailed experiment plans, discussions, and presentations. It is vital to strive to achieve the research objectives, but we will teach you to acquire the ability to evaluate the experimental results fairly.

[Job category of graduates] University faculty, postdoctoral fellow, patent examiner, Chemical/pharmaceutical industry

### **Research outline**

Our laboratory will develop functional biomaterials that can treat intractable diseases based on polymer science, biomaterials, drug delivery system (DDS) and regenerative medicine. In recent years, advanced medical treatments, including gene and cell therapy, have been implemented, and new treatment methods have been pioneered for diseases that have been considered incurable. Research on biomaterials that support such advanced medical treatment is expected to play an increasingly important role in the development of medical technology that will enable the treatment of intractable diseases in the future. We are developing research collaboration with overseas research institutes such as Singapore, Korea and the United States and promote research and development aimed at clinical application and industrialization.

### [Green tea catechin-based nanoparticles as DDS]

We have pioneered the design of nanoparticles comprised of green tea catechin derivatives for anticancer drug delivery. The green tea catechin has been shown to possess anticancer effects. The green tea catechin-based nanoparticle stably encapsulated anticancer proteins and achieved tumor-selective delivery, dramatically increasing anticancer efficacy from the combinational effects of the carrier and protein drugs, as compared to the drug alone (Fig. 1).

The high-performance drug carrier system of the nanoparticle is considered to enable a more effective and safer strategy for cancer therapy, suggesting a scope for an improved nano-medicine formulation. We will further develop the drug carrier system with green tea catechin derivatives to tackle intractable diseases, including cancer and other diseases.

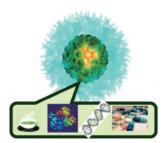


Fig.1. Green tea catechinbased nanoparticle for disease treatment

### [Injectable hydrogel system for biomedical applications]

We have developed the simple and biocompatible *in situ* gel-forming system composed of biodegradable polymer-phenol conjugates using a peroxidase-catalysed oxidation reaction (Fig. 2). This gel-forming system allows the formation of hydrogels without any inflammation and redundant reactions with bioactive agents loaded

in the hydrogels. In view of the injectable enzymatically crosslinked hydrogel system's promising properties, our hydrogel is expected to be an important tool in the field of biomaterial science and medicine. The research project involves controlled protein release from hydrogels, immuno-cancer therapy and 2/3D cell culture and differentiation control for cell therapy.

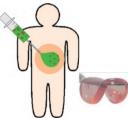


Fig.2. Injectable hydrogel system for biomedical applications

### Key publications

- N. Yongvongsoontorn, et al. Carrier-enhanced anticancer efficacy of sunitinib-loaded green tea-based micellar nanocomplex beyond tumor-targeted delivery, ACS Nano 13, 7591-7602 (2019).
- K. Liang, et al. Highly augmented drug loading and stability of micellar nanocomplexes comprised of doxorubicin and poly(ethylene glycol)-green tea catechin conjugate for cancer therapy, *Adv. Mater.* 30, 1706963 (2018).
- J. E. Chung et al. Self-assembled nanocomplexes comprising green tea catechin derivatives and protein drugs for cancer therapy, *Nature Nanotechnol.* 9, 907-912 (2014).

### Equipment

UV-visible spectroscopy, NMR, Dynamic light scattering, HPLC, Rheometer, Scanning electron microscope, Cell culture equipment, Animal research equipment

### **Teaching policy**

Our motto is to operate the laboratory in a style that is close to the students. We will strive to improve students' research abilities. When conducting applied research, we will thoroughly discuss the possibility of social contribution with students and provide an opportunity for students to develop their abilities to play an active role as leaders in society. We will expand students' potential by understanding their interests, abilities and individuality. While always being aware of the world's most advanced research, our laboratory is also on the stage, creating an atmosphere where students are intensely conscious of wanting to disseminate to the world.

### MAENOSONO Lab.

### Professor : MAENOSONO Shinya <sup>E-mail :</sup> shinya@jaist.ac.jp

[Research areas] Nanomaterials Chemistry; Colloid Chemistry [Keywords] quantum confinement effect; localized surface plasmon resonance; superparamagnetism; energy harvesting; nanomedicine; sensing

# Nanoparticle Science and Technology From Synthesis to Applications

Skills and background we are looking for in prospective students

Basic academic skills, communication ability, broad intellectual curiosity, flexible thinking

### What you can expect to learn in this laboratory

Nanoparticles have intermediate properties between atoms (molecules) and bulk crystals. We explore the frontiers of synthesis, higherorder structuring, and functionalization of nanoparticles. Our research in JAIST has focused on two main areas of interest in the field of materials chemistry and nanotechnology. The first area involved wet chemical synthesis of semiconductor nanoparticles with controlled size, shape and composition for energy conversion device applications. The second area has focused on the synthesis and biological application development of monometallic and alloyed multimetallic nanoparticles.

[Job category of graduates] Industry (chemical industries, precision equipment manufacturers, electronics companies, glass and ceramics companies, textile industries, etc.) and academic research institutes (universities, national institutes, etc.)

### **Research outline**

### 1. Thermoelectric nanoparticles

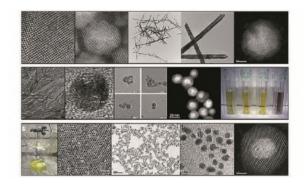
Thermoelectric materials have historically been an intriguing topic of materials science. In the global drive to develop sustainable energy, thermoelectric energy storage and generation technologies have attracted a tremendous interest. For practical applications, the dimensionless figure of merit,  $ZT=S^2 \sigma T/\kappa$  (S: Seebeck coefficient,  $\sigma$ : electrical conductivity,  $\kappa$ : thermal conductivity, T: temperature) is required to be higher than ca. 2. Unfortunately, the existing thermoelectric materials have much lower ZT value because of the interdependence of  $\sigma$  and  $\kappa$  which defines the limitation in the ZT value. It has been widely recognized that the nanostructured thermoelectric materials with well-defined nanoscale grain boundaries can have reduced  $\kappa$  without much decrease in  $\sigma$ . With this in mind, we are working on synthesis of thermoelectric materials.

### 2. Metal nanoparticles

Metal nanoparticles have long been utilized for various types of chemical and/or biological sensing applications. At the same time, much of the knowledge being gained for manipulating nanoparticle structure or composition has focused on multimetallic nanoparticles. Such systems can display multiple properties arising from the individual components, but it is the observation of synergistic phenomena that is the most intriguing. By taking advantage of such synergistic phenomena, one can enhance the sensing properties when these multimetallic nanoparticles are used as sensing probes. We focus on the synthesis of novel multimetallic heterostructured nanoparticles and their applications including, but not limited to, biosensing probes, chemical sensors, and nanocatalysts.

### 3. Magnetic nanoparticles

Magnetic nanoparticles show great potential for various bio-medical applications from diagnosis to therapy. Multifunctional heterostructured magnetic nanoparticles are quite interesting materials from fundamental and practical point of view. This class of hybrid magnetic nanoparticles include magnetic-fluorescent and magnetic-plasmonic bifunctional nanoparticles can offer new opportunities for biomedical applications. In our research, we synthesize magnetic nanoparticles, and then their surfaces are coated with semiconductor or plasmonic materials. For example, we created FePt@CdSe core@shell bifunctional nanoparticles which have magnetic and fluorescent properties stemming from FePt core and CdSe shell, respectively. In another case, we have synthesized Ag@FeCo@Ag double-shell bifunctional nanoparticles which combine magnetic and plasmonic properties. Those bifunctional nanoparticles can be used in wide range of biomedical applications.



### **Key publications**

- T. S. Le, M. Takahashi, N. Isozumi, A. Miyazato, Y. Hiratsuka, K. Matsumura, T. Taguchi, and S. Maenosono, "Quick and Mild Isolation of Intact Lysosomes Using Magnetic-Plasmonic Hybrid Nanoparticles", ACS Nano 16 (2022) 885
- 2. J. Hao, B. Liu, S. Maenosono, and J. Yang, "One-Pot Synthesis of Au-M@SiO<sub>2</sub> (M = Rh, Pd, Ir, Pt) Core-Shell Nanoparticles as Highly Efficient Catalysts for the Reduction of 4-Nitrophenol", *Sci. Rep.* **12** (2022) 7615
- 3. T. S. Le, S. He, M. Takahashi, Y. Enomoto, Y. Matsumura, and S. Maenosono, "Enhancing the Sensitivity of Lateral Flow Immunoassay by Magnetic Enrichment Using Multifunctional Nanocomposite Probes", *Langmuir* **37** (2021) 6566

### Equipment

TEM, STEM, XRD, XPS, NMR, ICP-OES, SQUID, PPMS, DLS, UV-Vis, TGA, Raman, *etc.* 

### **Teaching policy**

### [Website] URL: https://www.jaist.ac.jp/~shinya/

For students who go on to work in industry soon after graduation, I will cultivate a comprehensive ability and give overall guidance to enable them to smoothly receive job offers. For students who want to pursue a PhD, I will provide a leading-edge and international research environment to enable them to find a career in academia. Professor : MATSUMI Noriyoshi <sup>E-mail :</sup> matsumi@jaist.ac.jp

[Research areas] Creation of Energy Related Materials
[Keywords] Lithium ion secondary batteries, Metal-air batteries, Electrocatalysis (oxygen reduction, photoelectrochemical water splitting), Solid polymer electrolytes, Ionic liquids, Organoboron compounds/materials

# From Heteroatom Chemistry to Future Energy

### Skills and background we are looking for in prospective students

Aspiration, Intellectual Curiosity, Optimistic Character, Human skills to work in good harmony with other students/members If you have background in Organic Chemistry/Polymer Chemistry/Electrochemistry, it will be advantageous (not mandatory)

### What you can expect to learn in this laboratory

Skills to design, synthesize and characterize materials. Skills to objectively analyze the data and understand their significance properly. Skills to arrange short term/long term research schedule. Skills to give presentation, to discuss about research data. Skills to communicate with other laboratory members in English. More technically, students can acquire skills on preparation of organic compounds under inert atmosphere, characterization of the prepared compounds by NMR etc., evaluation of ionic conductivity by impedance measurements, evaluation of charge-discharge characteristics of Li ion battery cells, photo-electrochemical evaluation of electrocatalysts etc.

[Job category of graduates] Chemical companies, Polymer related companies, Printing companies, Mechanical companies etc.

### **Research outline**

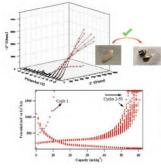
**1. Organic-inorganic hybrid electrolytes for battery safety** Design of non-flammable electrolytes are highly important class of materials for battery safety. By in-situ sol-gel condensation of alkoxysilane/alkoxyborane monomers in the presence of low viscous ionic liquids, we designed highly conductive ion-gel electrolytes which also exhibit thermal stability till 400°C . These electrolytes were used for fabrication of Li ion secondary battery cells, and the obtained cells showed reversible and satisfactory charge-discharge characteristics.

### Single ion conductive and electrochemically stable organoboron electrolytes

Ordinary electrolytes generally show very limited selectivity for lithium ion transport (lithium transference number). In order to enhance the lithium transference number, addition of Lewis acidic organoboron compounds to electrolytes is a valuable approach. Some classes of ionic liquids were found to be miscible with organoboron compounds, and binary mixture of ionic liquids/organoboron compounds were designed. In the presence of lithium salts, these system showed maximum lithium transference number of greater than 0.9, which is extraordinary high among liquid electrolytes. Moreover, these systems were also found to show high electrochemical stability. When these electrolytes are employed for Li ion secondary battery cell (Li/electrolyte/Si), maximum discharging capacity close to 3000 mAhg<sup>-1</sup> was observed.

### 3. Binder materials for high performance Li ion secondary batteries

In Li ion secondary batteries, PVDF have been widely employed as a binder material. However, PVDF is insulating in nature and fairly increasing the internal resistance of battery cells. We are designing electrochemically self-dopable conjugated polymer binders which shows remarkably reduced internal resistance after electrochemical cycles. This resulted in fairly improved discharging capacity of battery cells when compared with the case of PVDF binder.



#### Organic-inorganic hybrid non-flammable electrolytes

### Key publications

- "Extreme fast charging capability in graphite anode via lithium borate type bio-based polymer as aqueous polyelectrolyte binder", A. Pradhan, R. Badam, R. Miyairi, N. Takamori, N. Matsumi, ACS Materials Lett., 5 (2023) 413-420.
- "Enabling ultrafast charging in graphite anodes using BIAN-based conjugated polymer/lithium polyacrylate as a binder", SN. Mishra, S. Punyasloka, BS. Mantripragada, A. Pradhan, N. Matsumi. ACS Appl Ener Mater., 6 (2023) 11954-11962.
- "Charge–discharge behavior of lithium-ion batteries using a polymer electrolyte bearing high-density functional groups" A. Patra, N. Matsumi. ACS Appl Ener Mater., 6 (2023) 11973-11982.

### Equipment

Vacuum glove box, Impedance analyzer, Potentiogalvanostat, Cyclic voltammetry, Solar simulator, Gel permeation chromatography, Dynamic scanning calorimetry, Viscometer, Fluorescence spectrometer

### **Teaching policy**

#### [Website] URL: https://www.jaist.ac.jp/ms/labs/matsumi/english/index.html

On the basis of organic synthesis, we are working on challenging research fields of high social demands such as Li ion secondary battery, electrocatalysts for oxygen reduction reaction (fuel cell/metal-air batteries) and photo-electrochemical water splitting. We welcome students of various backgrounds such as organic chemistry, inorganic chemistry, electrochemistry, polymer chemistry, analytical chemistry, photo chemistry, device oriented materials engineering etc.



### MATSUMURA Lab.

### Professor : MATSUMURA Kazuaki <sup>E-mail :</sup> mkazuaki@jaist.ac.jp

[Research areas] Polymer Biomaterials. [Keywords] Polyampholytes, Zwitterionic polymers, Drug delivery system, Tissue Engineering, Hydrogels, Cryopreservation

# Functional polymeric biomaterials for controlling the functions of living systems



### Skills and background we are looking for in prospective students

Basic knowledge of chemistry is necessary for chemistry-based development of biomaterials that will be used in living organisms. This also entails knowledge of biology and medical science. The multidisciplinary approach must include chemistry and polymer chemistry.

### What you can expect to learn in this laboratory

Biomaterials research is an interdisciplinary activity that includes chemistry, biology, medicine, and physics. By learning about the highly controlled function of living organisms and continuing research aimed at creating materials to correct dysfunctional behaviors, a wide range of academic disciplines is covered. These include biology, medicine, physics, and chemistry.

Research on biomaterials is a need-oriented research whose purpose is clear, so it is possible to simultaneously foster problem-solving skills, which is especially valuable for PhD students.

[Job category of graduates] Chemical and Medical-device manufacturer, materials related companies

### **Research outline**

### **Functional Biomaterials**

The creation of functional polymers has been widely studied as an application in biomaterials and tissue-engineering materials. Functional polymers have many applications with regard to biomaterials. These include hydrogels, bioabsorbable materials, and artificial bones. Bulky soft materials and colloids, micelles, and even solutions can be studied as materials for controlling the functions of cells or tissues.

### **Cryoprotective Polymers**

Polyampholytes are polymers that have both positive and negative ions in the same molecule. We have demonstrated that several kinds of polyampholytes have a cryoprotective effect on cells in solution. This interesting phenomenon is a characteristic of polymers with high electron charge, especially polyampholytes. We will investigate and develop membrane-protective materials that can control cell functions by clarifying the mechanisms underlying such effects. Polyampholytes can change their conformation by controlling the polyion complex and thus exhibit various interesting physicochemical properties. We will try to develop novel functional materials by investigating the interactions between living systems and these polymers and by exploiting the physicochemical properties of the polymers.

#### **Tissue-Engineering Biomaterials and DDS Nanocarriers**

Biodegradable polysaccharide hydrogels for tissue engineering and drug delivery systems (DDS) are also being developed. We developed a novel degradation technique for dextran and cellulose by the addition of amine compounds, and elucidated the mechanisms of degradation. These biodegradable materials can be useful as cell scaffolds and drug-delivery nanocarriers.

#### **Biomaterials Well-matched to Living Systems**

We also perform basic and applied research on materials that are

well-matched to living systems. This research aims at regeneration of functions in tissue engineering. In particular, we are trying to

develop a novel cell culture scaffold and articular cartilage using hydrogels with high mechanical properties. The research being performed in our laboratory fuses chemistry and biology through polymer chemistry, toward the development of materials that can



Tissue engineering materials

Development of novel biodegradable cellulose for tissue enginee

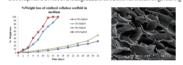


Figure. Examples of the research topics.

### **Key publications**

control living systems.

- Yamasaki R, Rajan R, Matsumura K. Enhancement of cryopreservation with intracellularly permeable zwitterionic polymers. Chem. Comm. 59, 14001-14004 (2023)
- Rajan R, Kumar N, Zhao D, Dai X, Kawamoto K, Matsumura K. Polyampholyte - Based Polymer Hydrogels for the Long - Term Storage, Protection and Delivery of Therapeutic Proteins. Adv. Healthc. Mater. 12, 2203253 (2023)
- Kumar N, Oqmhula K, Hongo K, Takagi K, Yusa S, Rajan R, Matsumura K. Mechanistic insights and importance of hydrophobicity in cationic polymers for cancer therapy. J. Mater. Chem. B, 11, 1456-1468 (2023)

### Equipment

UV-visible spectroscope, Fluorescence spectroscope, Cleanbench for cell culture, Incubator, Infrared resonance spectrometer, Differential scanning calorimeter, NMR

### **Teaching policy**

#### [Website] URL: https://matsu-lab.info/

In our laboratory, we attempt to understand the fundamentals and applications of polymer chemistry and aim to apply these fundamentals to biomaterials research. For this, we need to be familiar with a wide range of disciplines, such as chemistry knowledge, biology, medicine, mechanical engineering, and others. In addition, the range covered by biomaterials is diverse, such as artificial organs, regenerative medicine, drug delivery, and biosensors. We aim to acquire the knowledge necessary for research and development from a multilateral perspective. We also aim to nurture the problem-solving skills of our students. Students acquire presentation skills through several annual academic presentations and cultivate discussion abilities via a laboratory seminar once a week.

### MIYAKO Lab.

Professor : MIYAKO Eijiro

E-mail : e-miyako@jaist.ac.jp

 [Research areas] Bioengineering; Materials Chemistry; Nanotechnology; Nanomedicine
 [Keywords] Nanorobot; Nanobio; Nanomaterials, Bio-functional materials; Biotechnology; Biomimetics

# Creation of Game-Changing-Technology by Functional Materials and Bioengineering



### Skills and background we are looking for in prospective students

Special skills and background are not required at the beginning because you would be trained step-by-step after joining to the lab. We are looking for the students who really want to be a real scientist and an international first grade researcher and eager to learn something with flexible mind, cooperativeness, much curiosity, ambitious spirit to explore true natural science and new technology in various biological fields such as medical and agriculture with us all together.

### What you can expect to learn in this laboratory

Our research is fully multidisciplinary works and a sort of polyhedron prepared by our thinking and learning. Thus, you can learn anything if you want, for instance, organic syntheses, biochemistry, genetic engineering, skills for cellular and animal experiments, nanomaterials, medical device, robot and so on. Let's get started with us right now to carve up your own unique research by something you learned up to now!

### **Research outline**

Research interests of MIYAKO laboratory are in the area of bioengineering, materials chemistry, nanotechnology and nanomedicine. For example, using various physicochemical properties of nanomaterials, we challenge to develop an innovative nano-bio system that can monitor and control biological activities and health conditions at nanoscale level (Figure 1). For this objective, our work is also focused on the synthesis of high-quality "nanorobots", the engineering of their surface, and their assembly and consolidation into functional nanorobot to the aforesaid target biological applications, as well as to develop fundamental understanding of structure-property relationships.

We are also concentrating on creating nature-inspired materials and robotic engineering as game-changing technology in the field of food and agricultural industries (Figure 2). Our research is always based on the interdisciplinary nature with a lot of study fields such as chemistry, physics, biology, material science, and engineering etc..

### Past Representative Research Themes

- 1.Bioelectronic Implant Nanodevice
- 2.Liquid Metal Nanotrans former
- 3.Supramolecular Nanotrain
- 4.Nanomodulator for Cellular Stimulation
- 5.Photothermic Regulation of Gene Expression
- 6.Light and Magnetic Field-Driven Nanotransporter
- 7.Materially Engineered Artificial Pollinator (Robo bee)

They are just representatives. Our ultimate dream is to create the best science and technology in the world. Why not make an innovative technology and explore your own cool research field with us?

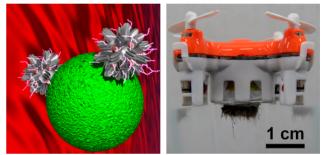


Figure 1. Schematic illustration of a Figure 2. Image of a bio-inspired robotic representative nanorobot for future bee for artificial pollination. innovative nanobiosystems.

### Key publications

- Yue Yu, Xi Yang, Sheethal Reghu, Sunil C. Kaul, Renu Wadhwa, Eijiro Miyako\*, "Photothermogenetic inhibition of cancer stemness by near-infrared-light-activatable nanocomplexes" Nature Communications 11, 4117 (2020).
- Svetlana A. Chechetka, Yue Yu, Xu Zhen, Manojit Pramanik, Kanyi Pu, Eijiro Miyako\*, "Light-driven liquid metal nanotransformers for biomedical theranostics" Nature Communications 8, 15432 (2017).
- Eijiro Miyako\*, Kenji Kono, Eiji Yuba, Chie Hosokawa, Hidenori Nagai, Yoshihisa Hagihara "Carbon nanotube-liposome supramolecular nanotrains for intelligent molecular-transport systems" Nature Communications 3, 1226 (2012).

### Equipment

Laser, fluorescent microscopy, UV-Vis-NIR spectrometer, fluorescent spectrometer etc.

### **Teaching policy**

### [Website] URL: https://e-miyakolab.amebaownd.com/

Here is English-based laboratory. We are willing to do my best as much as possible for your future scientific career and share with them the experimental analytical skills, the ability to think independently, express one's self logically, the capability to learn outside the traditional classroom setting and so on through discussion, journal club, annual meeting and conference. Especially, we will commit to the students, who would like to pursue a PhD, to enable them to find a research career in industry and academia by providing a cutting-edge and international research atmosphere with a lot of our collaborators all the world. Besides, our core-time of the laboratory is from 9am to 17pm except for one-hour break. Herein, we expect you must efficiently, effectively and speedy carry out works. Reflash after 17pm and holidays. In other words, study hard and play hard. Miyako laboratory will also actively develop and promote people from a variety of backgrounds who differ in terms of experience, knowledge, sensibility, perspective, cultural background, and values, and in so doing will not discriminate based on ethnicity, nationality, gender, religion, age, social position, or disability.

### MURATA Lab.

Professor : MURATA Hideyuki <sup>E-mail :</sup> murata-h@jaist.ac.jp

[Research areas] Optoelectronic devices based on organic semiconductors [Keywords] Organic Light Emitting Diodes, Organic Solar Cells, Organic Field Effect Transistors, Operando measurements, Exciton dynamics in organic semiconductors

# Development of High Performance and Stable Organic Electronic Devices



### Skills and background we are looking for in prospective students

We are looking for students who are curious to develop optoelectronic devices based on organic materials. By considering your research experience and scientific background, we will determine your research project.

### What you can expect to learn in this laboratory

You will learn fabrication techniques of organic devices using vacuum deposition method or solution process (spin-coating, dip-coating). You will also learn characterization skills of organic devices using several electrical and optical measurements. Besides experimental skills, you may learn fundamental sciences related to organic devices including device physics, materials science and photochemistry. You will also learn essential skills required as a researcher, such as management of research, documentation and presentation skills.

[Job category of graduates] Researchers and engineers in electronics, chemical, machinery, battery industries, and faculty member in university and national institutes

### **Research outline**

We have been working on organic electronics, such as organic light emitting diodes (OLEDs), organic solar cells, and organic memory. Professor Murata is interested in elucidating the degradation mechanism of OLEDs and developing new optoelectronic devices. Assistant Professor Eguchi is developing in-situ observation methods and measurement methods under operating environments. He is also conducting research on enhancing device performance of various devices and their mechanisms by surface and interface modification.

### Elucidation of degradation mechanism of OLEDs

OLED displays provide the best image quality and they can also be made transparent, flexible, foldable and even rollable and stretchable in the future. The most important challenge in the current OLED field is to achieve high efficiency and durability in blue OLEDs. We are elucidating the degradation mechanism of blue OLEDs using fluorescent, phosphorescent and thermally activated delayed fluorescent materials. We have excellent research facilities to fabricated OLEDs and to characterize the devices by electrical and optical measurements.

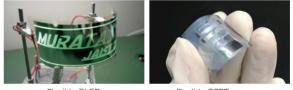
### Evaluation of structures and electronic states under device operation

We have recently started the development of Operando measurement systems to evaluate structures and electronic states of molecular thin films in actual organic devices under working conditions. These new measurement techniques enable us to deepen our understanding of device physics and to improve device characteristics. We are also planning to develop a new method to measure physical properties of thin films in situ during device fabrication process, and aim to develop high-performance organic devices.

### Organic memory

We are trying to realize a non-volatile organic memory with a new

operating mechanism that takes advantage of the characteristics of organic materials. We are developing new materials for 2-terminal devices with simple structures and 3-terminal devices based on transistors.



Flexible OLED

Flexible OFET memory

### **Key publications**

- D. C. Le, D. D. Nguyen, S. Lloyd, T. Suzuki and H. Murata, Degradation of fluorescent organic light emitting diodes caused by quenching of singlet and triplet excitons, J. Mater. Chem. C, 8, 14873 (2020)
- T. T. Dao, H. Sakai, K. Ohkubo, S. Fukuzumi, H. Murata, Low switching voltage, high-stability organic phototransistor memory based on a photoactive dielectric and an electron trapping layer, Organic Electronics 77C, 105505 (2020).
- V. Vohra, K. Kawashima, T. Kakara, T. Koganezawa, I. Osaka, K. Takimiya, H. Murata, Efficient inverted polymer solar cells em- ploying favourable molecular orientation, Nature Photonics, 9, 403 (2015).

### Equipment

Ultra-high vacuum depositing system,

High vacuum deposition system with glove box

Device characterization system

Photoluminescence quantum yield measurement system, Time-resolved photoluminescence and electroluminescence measurement system

Device stability measurement system

Photoelectron yield spectroscopy, Inverse photoelectron spectroscopy

### **Teaching policy**

#### [Website] URL: https://www.jaist.ac.jp/ms/labs/murata/index.html

During undergraduate education, you may have learnt basic knowledge of your field of expertise. A graduate school is a place to carry out your research using your knowledge with acquiring advanced knowledge. Even if your research goes wrong and you face obstacles, the experience of overcoming difficulties is valuable. I think that a successful experience gives you confidence, and overcoming difficulties bring up you to the next stage.

### NAGAO Lab.

### Professor: NAGAO Yuki

E-mail : ynagao@jaist.ac.jp

 [Research areas]
 Protonics, Polymer Chem., ElectroChem. Coordination Chem., Surface Chem.

 [Keywords]
 Proton Conductive Materials, Self-assembly, Electrochemical Catalysts, Fuel Cells, Energy Conversion, Sensors, Battery

# Innovating for a Greener Future through Advanced Materials Science



### Skills and background we are looking for in prospective students

Our group respects your diverse research background. We are looking for students who can keep a high motivation to tackle new research while demonstrating your strengths. It is vital to create a laboratory where research staff and students can share the spirit of co-prosperity.

### What you can expect to learn in this laboratory

Through twice a week seminars conducted in English, specifically research discussion and literature introduction, you will acquire the ability to examine and think oneself, with the help of supervisor and seniors. As a practice opportunity, you will study on polymer chemistry, surface chemistry, electrochemistry, coordination chemistry etc. You also acquire following things. 1. Problem discovery and solution method. 2. Material synthesis and various analytical methods. 3. Interpretation method of data based on logical thinking and presentation skill.

[Job category of graduates] University faculty in home country, Chemical company, Energy company

### **Research outline**

Securing diverse energy resources is an urgent issue for resource-poor Japan to achieve sustainable development. And it is a dream of mankind to create hydrogen and oxygen from common water, and to create carbon materials using carbon dioxide as a resource. A hydrogen society is necessary for the decarbonized society that is rapidly progressing in the world. We are researching ion-conducting polymer materials, inorganic materials, and organic-inorganic hybrid materials using interfaces that can be applied to fuel cells, batteries, and sensors that support the hydrogen society. Let's contribute to a hydrogen society together with us.

### **Research Themes**

- 1. Research on fuel cell performance improvement Proton transport property in polymer organized structure OH<sup>-</sup> ion transport property in polymer thin films
- 2. Research on Li ion battery performance improvement Precise polymer arrangement for electrolyte-electrode interface
- 3. Rechargeable proton batteries
- 4. Research on external force response sensors using ion transport
- 5. Ion switching by coordination compounds (Dr. Aoki, Assistant Professor)



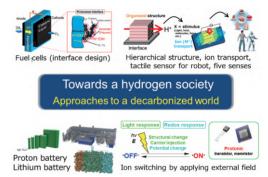


Fig. 1 Schematic of our research. Materials science for development of polymer electrolyte fuel cells, batteries, tactile sensor, and ion switching.

### **Key publications**

- Y. Yao, H. Watanabe, M. Hara, S. Nagano, Y. Nagao, Lyotropic Liquid Crystalline Property and Organized Structure in High Proton-Conductive Sulfonated Semi-Alicyclic Oligoimide Thin Films, *ACS Omega*, 8, 7470 - 7478 (2023).
- F. Wang, S. Nagano, M. Hara, Y. Nagao, Hydration and OH<sup>-</sup>/Br<sup>-</sup> Conduction Properties of Fluorene-Thiophene-Based Anion Exchange Thin Films Tethered with Different Cations, *ACS Appl. Polym. Mater.*, **4**, 5965 - 5974 (2022)
- F. Wang, D. Wang, Y. Nagao, OH<sup>-</sup> Conductive Properties and Water Uptake of Anion Exchange Thin Films (Selected as The Cover Feature), *ChemSusChem*, **14**, 2694 - 2697 (2021).

### Equipment

Material analyzer (IR, UV-Vis, NMR, GPC, XRD, TG-DTA) Electrochemical equipment (LCR, CV, in situ QCM, fuel cell, battery test system) Surface analyzer (XPS, in situ GIXRS, XRR, white interference, AFM) Molecular orientation analyzer (IR, pMAIRS, polarized microscope) External synchrotron and neutron experiments

### **Teaching policy**

#### [Website] URL: https://www.jaist.ac.jp/ms/labs/nagao-www/?lang=en

We do not set core time, but encourage you to do experiments basically from 9am to 5pm. The research topic will be determined in consultation with the research staff. We expect the following to our students: 1) to learn through cutting-edge research; 2) to improve your communication skills to facilitate your research; 3) to refresh as much as possible on weekends for leading a fulfilling life; 4) to actively interact with outside researchers.

Seminars are held twice a week, research discussion and journal paper introduction meetings. Once a month, a joint presentation meeting is held with laboratories from other universities. Conference presentations and publications are encouraged. Financial support is provided for contributions to laboratory operations and collaborative research.

## OHDAIRA Lab.

Professor: OHDAIRA Keisuke <sup>E-mail:</sup> ohdaira@jaist.ac.jp

[Research areas] Solar cells, Semiconductor engineering, Thin film formation [Keywords] crystallization, passivation, module reliability

# Develop next-generation Si-based solar cells through novel process technologies

### Skills and background we are looking for in prospective students

Students are preferred to have basic knowledge of solid-state physics and semiconductors. Concerns for a global environmental issue and an energy problem may become a driving force to promote their research.

### What you can expect to learn in this laboratory

Students can achieve skills for the operation of vacuum equipment, thin-film formation and characterization, device fabrication and characterization by performing their own research. They can also acquire basic academic skills for semiconductors and solar cells through data analysis, daily discussion, and a weekly seminar. Furthermore, students can gain high problem-solving skills, owing to the policy of our group supporting individual initiatives. Presentation and communication skills can be strengthened through presentations in domestic and international conferences and a booth exhibition.

[Job category of graduates] Post-doctoral researcher in institutes, Manufacture and research work of electronics and materials related companies

### **Research outline**

Solar cells based on silicon, which is highly abundant on the earth, dominate the present market share of photovoltaic technologies, and is expected to be the leading player also in the future. At the same time, the development of solar cells with lower cost, higher efficiency, and long-term reliability are necessary, and further technological breakthroughs are required. Our group focuses on the following research topics and attempts to establish the basic technology of silicon-based high-performance solar cells.

### 1. Formation of polycrystalline silicon films for solar cells by rapid annealing

Flash lamp annealing (FLA), millisecond-order discharge from Xe lamps, can supply pulse light with a fluence of several tens of  $J/cm^2$ , which momentarily corresponds to several tens of thousands times as much as sun-light on the earth. Our group investigates the formation of polycrystalline silicon (poly-Si) films on low-cost glass substrates for cost-effective solar cells. Poly-Si films with a thickness of >4 µm can be formed by supplying a single shot of flash lamp pulse on precursor amorphous silicon (a-Si) prepared on glass substrates. When hydrogenated a-Si films are used as precursor films, hydrogen atoms remain inside the silicon films even after crystallization, which can contribute to the termination of dangling bonds in the poly-Si and the formation of poly-Si films with low defect density. Our group investigates the fundamental mechanism of the crystallization of a-Si films by FLA and the application of the poly-Si films to thin-film crystalline silicon solar cells.

### 2. Application of catalytic chemical vapor deposition (Cat-CVD) to the fabrication of solar cells

Cat-CVD, a film deposition method through the catalytic cracking of gas molecules on a heated catalyzing wire, can reduce damage to a sample surface due to its plasma-damage-less nature, and can produce high-quality passivation films which can significantly suppress the recombination of minority carriers on the surface of crystalline silicon and lead to the realization of high-efficiency crystalline silicon solar cells. Cat-CVD apparatus can also be utilized for the doping of B or P atoms to the surface of silicon samples by exposing to B- or P-related radicals formed by the catalytic cracking of  $B_2H_6$  or  $PH_3$ . This novel process, catalytic impurity doping (Cat-doping), can be applied to the formation of front- or back-surface field layers and doping layers in crystalline silicon solar cells.

### 3. Reliability and novel structure development of crystalline silicon photovoltaic modules

The performance degradation of photovoltaic modules owing to a voltage between a module frame and cells, potential-induced degradation (PID), is a crucial issue particularly in large-scale photovoltaic power plants in which a number of cells and modules are connected in series. We investigate the mechanism of the PID of crystalline silicon photovoltaic modules and develop measures for the suppression of the PID. In addition, components in the present conventional modules are adhered with encapsulant. This causes various types of degradation originating from the encapsulant and makes it difficult to sort and recycle the components when disposing of the modules. To solve this problem, we are also developing new-type photovoltaic modules with no encapsulant.

### Key publications

- K. Ohdaira, M. Akitomi, Y. Chiba, and A. Masuda, Potential-induced degradation of n-type front-emitter crystalline silicon photovoltaic modules — comparison between indoor and outdoor test results, Sol. Energy Mater. Sol. Cells 249, 112038 (2023).
- H. T. C. Tu and K. Ohdaira, Long term stability of low temperature deposited Cat-CVD SiNx thin film against damp-heat stress, Jpn. J. Appl. Phys. 63, 01SP25 (2024).
- Z. Wang, H. T. C. Tu, and K. Ohdaira, Crystallization of catalytic CVD hydrogenated n-a-Si films on textured glass substrates by flash lamp annealing, Jpn. J. Appl. Phys. 61, SB1019 (2022).

### Equipment

FLA system Cat-CVD chamber Solar cell characterization system Photovoltaic module fabrication and characterization system Thin-film characterization system

### **Teaching policy**

#### [Website] URL: https://www.jaist.ac.jp/ms/labs/ohdaira/en/home\_e

Our group has a policy of supporting students' individual initiatives, and their own ideas can be included in their researches. A morning meeting is held every weekday, and the activities of each student are shared. Students can also have simple research discussion in the meeting. In a study meeting, held on every Saturday, a duty student is required to explain the detail of a journal paper and to answer questions from other students and staffs, by which students can obtain high basic academic skills. Students can actively present their research achievements, and acquire ability to write their own research paper for themselves.



# OHKI Lab.

### Professor: OHKI Shinya

[Research areas] Protein NMR [Keywords] Protein, Structure-function relationship, NMR

E-mail :

shinya-o@jaist.ac.jp

# Exploring structure-function relationship of proteins using NMR spectroscopy



To start the research work at my group, students should have at least one of the basic knowledge of biochemistry, biotechnology, bioinformatiocs and NMR at undergrad level. The students who are good at computer work are also welcome.

### What you can expect to learn in this laboratory

The goal of our research work is understanding biological functions of proteins at molecular level based on their three-dimensional structures and dynamics. For this purpose, we are employing modern NMR techniques. My group is the super-user of four NMR machines (400MHz x 2, 500MHz, and 800MHz) in JAIST, thus the students in my group are expected to be NMR experts. Because we are working on biomolecules, a wide variety of skills for preparing and analyzing them will also be acquired. Scientific writing, presentation and discussion skills are of course trained at group meeting and conferences.

[Job category of graduates] R & D of food, chemical, and pharmaceutical companies

### **Research outline**

### (1) Development of stable-isotope labeling methods

Protein NMR samples are necessary to be labeled with NMR active nuclei, such as <sup>13</sup>C and <sup>15</sup>N. Techniques for preparing such NMR samples are called as "stable-isotope labeling". The labeling is normally achieved by using genetically modified *E. coli.*, but not all protein samples can be expressed by *E. coli.* Thus, many other methods have been proposed. As one of the alternatives, we had developed a method to use plant BY2. Because BY2 is a higher cell, it has a potential to express complex proteins which are difficult for *E. coli.* to synthesize. Moreover, using BY2, we had optimized the protocol for labeling only lle, Leu, and Val residues in the sample protein. We are continuously trying to develop some new labeling methods using the BY2 system.

### (2) Proteins and peptides containing disulfide bonds

It is difficult for *E. coli* system to express proteins and peptides containing disulfide bonding (SS-bond). However, the BY2 system can do it. Thus, we have been trying to explore structure-function relationship of proteins and peptides containing SS-bonds. Here two topics what we had done are described briefly for your better understanding. Stomagen, one of the peptide hormones, increases stomatal density of plants. Because stomagen contains three SS-bonds, sufficient amount sample was not prepared using *E. coli* system. We, however, could prepare the stable-isotope labeled stomagen using the BY2 system, and studied its structure and dynamics. The NMR results opened the discussion for understanding structure-function relationship of the family members at atomic resolution. Until today, we have successfully designed and actually prepared the mutants showing desired bioactivity to increase or decrease the stomatal density. It is believed that such basic science will contribute to solve recent issues on food yield and earth environment in the future.

ESF, containing four SS-bonds, acts at the early phase in seed development. When ESF is inactive, the size and shape of seeds become heterogeneous. We have solved the three-dimensional structure of ESF prepared by the BY2 system. And the structure has indicated the key residues for its activity. It is expected that controlling the ESF activity might provide many applications to harvest big seeds for agriculture and fruits without seeds for easy food processing, etc.

We are also handling various other proteins and peptides containing SS-bonds, such as defensins and toxins. Knowledge of their structure-function relationship will help for developing new drugs.

### (3) Proteins in the signaling pathways

A wide variety of biological signals in cells is harmonized by proteins, lipids, nucleotides, etc. Post-transcription modification including phosphorylation and methylation is known as one of the cues for activating/inactivating the biological functions. The chemical modification is a trigger for structural change, resulting the new conformer interacting with the target molecule. We are focusing on monitoring the conformational transition of the proteins at work.



 Figure. (left) Three-dimensional (right) Methyl region of <sup>1</sup>H-<sup>13</sup>C CT-HSQC of BPTI.

 structure of stomagen.

 Leu and Leu/Val selective labeling are achieved.

### **Key publications**

- T. Imamura, H. Takagi, A. Miyazato, S. Ohki, H. Mizoguchi & M. Mori "Isolation and characterization of the betalein biosynthesis gene involved in hypocotyl pigmentation of the allotetraplois Chenopodium quinoa" Biophys. Biochem. Res. Commun. (2018) 496, 280-286.
- L.M. Costa, E. Marshall, M. Tesfaye, K.A.T. Silverstein, M. Mori, Y. Umetsu, S.L. Otterbach, R. Papareddy, H.G. Dickinson, K. Boutiller, K.A. VandenBosh, S. Ohki & J.F. Gutierrez-Marcos "Central cell-derived peptides regulate early embryo patterning in flowering plants" Science (2014) 344, 168-172.
- S. Ohki, M. Takeuchi & M. Mori "The NMR structure of stomagen reveals the basis of stomatal density regulation by plant peptide hormones" Nat. Commun. (2011) 2, 512.

### Equipment

(in my group) deep-freezers, PCR, UV meter, centrifuges, bio-shakers, incubators, HPLCs, Linux machines, SPR, etc. (open facility) 800MHz-NMR equipped with a TCI cryogenic probe, MALDI-TOF/TOF MS, FT-MS, etc.

### Teaching policy [Website] URL : https://www.jaist.ac.jp/nmcenter/labs/s-ohki-www/contents/Ohki\_Lab.html

For the better scientific research work, discussion based on the experimental results is an undoubted important factor. Thus, students are recommended to discuss each other. And students can have opportunity to talk about his/her research progress at group meeting. Through the research, students get the knowledge how to plan small projects and to organize them toward the big goal.



Professor : OSHIMA Yoshifumi <sup>E-mail :</sup> oshima@jaist.ac.jp [Research areas] TEM/STEM, nanomaterials

# Nano-Characterization for innovation - In-situ TEM/SEM Observation -



### Skills and background we are looking for in prospective students

Our laboratory studies electrical, mechanical or electrochemical properties of nanomaterials, which has been pointed out to be strongly correlated with their atomic structures or shapes, using transmission electron microscope. Those who really want to find something new in nanomaterials' properties will be able to achieve such experiments. Your motivation and/or will are critical for accomplish your research project. If possible, you had better understand the fundamentals of mathematics and physics.

### What you can expect to learn in this laboratory

You will understand fundamentals of solid state physics deeply through experiments. The TEM image is information in real space and the diffraction is information in reciprocal space. Both informations are investigated in order to clarify the atomic structure of the sample, which make you understand the relationship between real and reciprocal spaces deeply. Also, you will master good skills, for example, TEM operation, Vacuum equipment operation, programming (LabView) and so on. Furthermore, you will be able to develop in-situ TEM holder by yourself, if you join the doctoral course, which is great advantage for you.

[Job category of graduates] Manufacture, Analytics company, Research laboratory

### **Research outline**

We have developed an experimental system of combining an atomic force microscope (AFM) with ultra-high vacuum transmission electron microscope (TEM) (see Figs. 1 and 2). Using this system, we can directly obtain relationship between atomic structure and mechanical strength of nano-scaled material. Such an experimental system is quite unique in the world and advantage for us.



Fig. 1 A photo of ultra-

high vacuum TEM. Only

a few UHV-TEM works in

the world.



Fig. 2 A photo of a AFM holder, which can be installed in the TEM. We developed such in-situ TEM holder by ourselves

We mainly use TEM and/or STEM, because these are powerful tools to observe materials at an atomic scale (see Fig. 3). We have found that very thin metal nanoparticles showed different structural phases from their bulk crystal structure and also very thin metal nanowire became tubular structure like carbon nanotube, for example. Recent advanced TEM enables us to visualized light element at an atomic scale.

We will devise unique experimental systems based on TEM and clarify relationship between atomic structure and physical and/or chemical properties of frontier materials. Our final goal is discovery of frontier materials, which is based on understanding physical and/or chemical properties at an atomic scale.

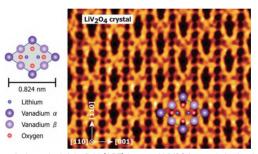


Fig. 3 A typical annular bright field (ABF) image of LiV2O4 crystal viewing from the [110] direction. Lithium ions are visualized in the image

### **Key publications**

- 1. J. Zhang, et al.,"Atomic scale mechanics explored by in situ transmission electron microscopy with a quartz length-extension resonator as a force sensor", Nanotechnology 31 (2020) 205706.
- 2. C. Liu, et al.,"Origin of nonlinear current-voltage curves for suspended zigzag edge graphene nanoribbon", Carbon 165 (2020) 476
- 3. Y. Chiew, et al.,"Ordering of Intercalated Fe Atoms in FexTiS2 Structures Clarified using Transmission Electron Microscopy", J. Phys. Soc. Jpn. 89 (2020) 074601.

### Equipment

Ultra High Vacuum Transmission Electron Microscope In-situ TEM holder (home-made) Vacuum chamber Frequency Modulation Atomic Force Microscopy Controler

### **Teaching policy**

#### [Website] URL: https://www.jaist-oshima-labo.com/english/

We held a regular meeting every week, in which we read a selected paper, discuss about research progress of assigned student and lean the fundamental of solid state physics with each other. I recommend mutual learning and/or discussion (a student teaches the others and vice versa) in order to understand solid state physics deeply. I also recommend that students attend domestic or international meetings and have presentations in order to improve communication skill.

### SUZUKI Lab.

Professor : SUZUKI Toshi-kazu <sup>E-mail :</sup> tosikazu@jaist.ac.jp

[Research areas] Compound semiconductor electronics [Keywords] Compound semiconductors, High-speed devices, Energy-saving devices, Device characterization

# Compound semiconductor devices for functional diversification of electronics



Fundamental understandings of physics/mathematics with logical abilities are important, although they are not necessary conditions.

### What you can expect to learn in this laboratory

Acquiring compound semiconductor device fabrication and characterization/measurement technologies, it will be possible to physically consider and understand the behavior of electrons in devices. This will be the foundation for future activities in various fields of electronics. In addition, it is encouraged to join collaborative research programs with industry, in order to have a firsthand knowledge of industrial electronics. We also place the importance of presentation skills.

[Job category of graduates] Electric appliance, Semiconductor device and electronic component, Semiconductor manufacturing equipment, Information and communication, Automotive

### **Research outline**

### Functional diversification of electronics

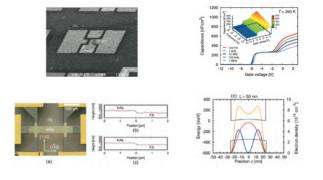
The "More Moore" paradigm based on Si-device scaling is facing fundamental limitations. In order to develop future electronics, functional diversification from the viewpoint of "More than Moore" is quite important. Compound semiconductor devices will play important roles towards such functional diversification.

### Why compound semiconductors?

There are various compound semiconductors with various physical properties, which are beneficial for various device functions. In particular, compound semiconductors with excellent electron transport properties and/or those with direct energy bands are suitable for excellent electron devices and/or optical devices. Narrow-gap compound semiconductors exhibiting high electron mobilities and high electron saturation velocities, such as InAs, are useful for high-speed device applications. Also, narrow-gap compound semiconductors having energy gaps corresponding to mid-infrared (MIR) light can be applied to optical devices in the MIR range. On the other hand, wide-gap compound semiconductors, such as GaN and AIN, have energy gaps corresponding to ultraviolet (UV) light, which are beneficial not only for UV optical device applications, but also for high-power electron device applications because of their high breakdown voltages. Since GaN exhibits a high electron saturation velocity owing to its large optical phonon energy and band structure, although its electron mobility is not so high, we can expect excellent high-speed, high-power, and energy-saving performances of GaN-based devices.

### Our researches

Towards functional diversification of electronics, it is important to use compound semiconductors "in the right material in the right place". Our laboratory is engaged in researches on compound semiconductor devices aiming at future high-speed and energy-saving applications. We develop device fabrication technologies using narrow- and wide-gap compound semiconductors. Moreover, device characterization/measurement technologies are developed in order to obtain deeper insights into device operations.



### Key publications

- Low-frequency noise in AlTiO/AlGaN/GaN metal-insulator-semiconductor field-effect transistors with non-gate-recessed or partially-gate-recessed structures, D. D. Nguyen, Y. Deng, and T. Suzuki, Semicond. Sci. Technol. 38, 095010 (2023).
- Mechanism of low-temperature-annealed Ohmic contacts to Al-GaN/GaN heterostructures: A study via formation and removal of Ta-based Ohmic-metals, K. Uryu, S. Kiuchi, T. Sato, and T. Suzuki, Appl. Phys. Lett. 120, 052104 (2022).
- Electron mobility anisotropy in InAs/GaAs(001) heterostructures, S. P. Le and T. Suzuki, Appl. Phys. Lett. 118, 182101 (2021).

### Equipment

Molecular beam epitaxy system Electron-beam/UV lithography systems Semiconductor parameter analyzer Network analyzer Dynamic signal analyzer

### **Teaching policy**

- ·Engineering with a scientific mind
- •Step-by-step with being convinced
- •Good collaboration between faculty and students
- •Creating a basis for future electronics

#### [Website] URL: https://www.jaist.ac.jp/nmcenter/labs/suzuki-www/



### TAKAMURA Lab.

Professor : TAKAMURA Yuzuru <sup>E-mail :</sup> takamura@jaist.ac.jp

[Research areas] BioMEMS, Microfluidics, Analytical Chemistry, Biosensor [Keywords] Blood analysis chip, Single cell analysis, Mass spectroscopy chip, Micro/Nano process, PZT Low-T process, Micro plasma

# Microfluidic devices and sensors for biochemical and medical applications

### Skills and background we are looking for in prospective students

The subjects we have been dealing with are strongly interdisciplinary fields, so we welcome students from various backgrounds. We will assign research topics according to individual background/interest such as physics, machinery, electronics, control, materials as well as advanced nano-biochemistry technologies.

### What you can expect to learn in this laboratory

Basic and practical skills in analytical chemistry. Some parts of our laboratory are closely related to molecular biology and/or materials science. Since we handle trace amount of sample so that students will learn a handling technique of trace amount of biological sample, interfacial treatment/integration between biomolecules and inorganic materials, observation / measurement technology of minute fluorescence and optical signal etc. In addition, you can also learn advanced micro/nanofabrication techniques, numerical simulation, material analysis methods such as TEM, SEM, XRD, XPS throughout your study.

[Job category of graduates] Analytical, electronics, mechanics, equipment manufacturer, semiconductor manufacturer, materials science/engineering, chemical related.

### **Research outline**

We are studying next generation biochip techniques for various biomedical and environmental applications, employing semiconductor technology, nanomaterials / biomolecules, micro / nanofluidcs, and lab-on-a-chip techniques. Our interest extends to a wide range in fusion of nanotechnology and biotechnology, understanding of phenomena in the nano & micro scale, and practical applications such as high sensitive point of care biosensors, manipulation of liquids on chip, analysis of single cell and single molecules, LEP-AES ultra-compact elemental analyzer, and various bio/chemical processing units.

### 1) Development of highly integrated biochemical chip

To realize a high-performance biochip, precisely fluid control on chip and highly sensitive detector are important.

In this laboratory, we are developing various liquid control mechanisms on chips including PZT actuator array by a solution process and novel detection technologies using nanomaterials and nanoscience (Fig.1). Using these, we aim to develop chips for single cell analysis in tissue at the molecular level, highly integrated biochip for general purposes (Fig.2).



Figure 1. Integrated microfluidic sensor and actuators.



### Development of highly sensitive biosensing technologies

A drop of blood contains rich information Figure 2. Concept model of total integrated microfluidics devices. body. Analyzing these enables various things, such as ultra-early detection of severe diseases, day-to-day health management, or guiding meals and

exercise avoiding lifestyle disease. To do this, we are developing various technologies to measure very small biomarkers with low-cost and user-friendly, including mass analysis chip, lab-on-paper, fully automated electrochemical sensors with fg/ml order limit of detection with comparable levels of cost and handling like SMBG (self-monitoring of blood glucose).

### Development of hand-held elemental analyzer using micro liquid electrode plasma

By simply putting a liquid sample into a micro channel whose center is made narrower and applying high voltage from both ends, we found that quantitative and highly sensitive measurement of trace amount of elements is possible from the emission of the generated plasma. Using this principle, we are developing micro elemental analyzer that can measure on-site harmful metals (Hg, Cd, Pb, etc.) contained in food, tap water, soil factory wastewater / waste.

### Key publications

- Pulse-heating ionization for protein on-chip mass spectrometry, Kiyotaka Sugiyama, Hiroki Harako, Yoshiaki Ukita, Tatsuya Shimoda, Yuzuru Takamura, Analytical Chemistry, 86, 15, 7593-7597, 05 August 2014.
- Development of automated paper-based devices for sequential multistep sandwich enzyme-linked immunosorbent assays using inkjet printing, Amara Apilux, Yoshiaki Ukita, Miyuki Chikae, Orawom Chilapakul and Yuzuru Takamura, Lab Chip,13(1), 126-135, January 2013.
- High sensitive elemental analysis for Cd and Pb by liquid electrode plasma atomic emission spectrometry with quartz glass chip and sample flow, Atsushi Kitano, Akiko liduka, Tamotsu Yamamoto, Yoshiaki Ukita, Eiichi Tamiya, Yuzuru Takamura, Analytical Chemistry 83(24), 9424-9430, 04 November 2011.

### Equipment

Clean Room and Semiconductor Fabrication Facility Electrochemical Equipment Surface Plasmon Resonance Equipment Total Reflection single molecule microscope Nano-imprinting systems

### **Teaching policy**

[Website] URL: https://www.jaist.ac.jp/ms/labs/takamura/index\_e.html

Many of the recent new technologies in medicine and life sciences are based on the advancement of new engineering technologies, especially fusion of nanotechnology and biotechnology. We are welcoming students having various backgrounds such as biology, physics, mechanics, electronics, and chemistry. We set goals according to each student's background and purpose, and support and guide them to acquire what they need towards them.



## TANIIKE Lab.

Professor: TANIIKE Toshiaki E-mail : taniike@jaist.ac.jp

[Research areas] High-throughput experimentation, materials informatics, computational chemistry [Keywords] Heterogeneous catalysis, polymerization, nanocomposites, membranes, graphene, data science

# Advanced Material Design based on Exploration, Learning, and Prediction



Our research areas are highly multidisciplinary, where students from various backgrounds, not only chemistry (catalysis, polymer, nanomaterials, etc.) but also engineering, data science, computation, and so on, are welcome.

### What you can expect to learn in this laboratory

Students will acquire 1) advanced research methodologies based on high-throughput experiments, data science, and computational chemistry; 2) a method of strategic planning for maximizing research outcome with given resources; 3) skills to work in an interdisciplinary and international environment.

[Job category of graduates] R&D for materials science, chemistry, chemical engineering

### **Research outline**

Facing rapid acceleration in science and technology, Taniike laboratory aims to develop and implement innovation-oriented materials science based on high-throughput experimentation (HTE), data science (materials informatics), and simulation. We explore a wide range of materials and provide solutions to the challenges of our society with unprecedented efficiency.

### 1. High-throughput experimentation

Combination of different elements and materials can bear an astronomical number of possibilities. One of the purposes in materials science is to discover good combinations and a novel way (process) to produce the combinations. We perform HTE using highly automated and/or parallelized instruments. We maximize the throughput of the experiments and change the research style from labor-intensive to brain-intensive works.

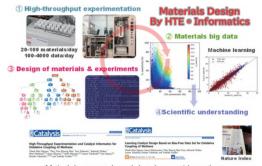
### 2. Data science

HTE generates materials big data which include synthetic conditions, structural characteristics, and performances of the materials. In order to implement efficient exploration of materials, it is not enough only to pick up good ones: It is necessary to clarify a structure-property relationship. Based on approaches of data science and materials informatics, we extract knowledge from the data and further accelerate materials discoveries.

### 3. Simulation

Developments of computers and computational chemistry have enabled realistic simulation of complicated materials. Nonetheless, virtual materials design in computers (i.e. in-silico design) is still far to be practical. The most difficult task is how to obtain a molecular model which represents a material. We use experiments and simulations in a comprehensive fashion for establishing a high-precision molecular model towards in-silico materials design. Computational chemistry based on deep understanding of experimental materials science is aimed.

Together with HTE instrumental development and data science programming, we focus on five subjects: Catalyst & polymer informatics; structure-performance relationship; nanomaterials like MOF, graphene; polymer nanocomposites.



Materials research and development based on high-throughput experimentation and materials informatics

### **Key publications**

- L. Takahashi, T. Taniike, K. Takahashi et al., Constructing Catalyst Knowledge Networks from Catalysts Big Data in Oxidative Coupling for Methane for Designing Catalysts, Chemical Science 2021, 12, 12546-12555 (press released, selected as Front Cover).
- T.N. Nguyen, K. Takahashi, T. Taniike et al., High-Throughput Experimentation and Catalyst Informatics for Oxidative Coupling of Methane, ACS Catalysis, 2020, 10, 921-932 (press released).
- G. Takasao, Toru Wada, T. Taniike et al., Machine Learning-Aided Structure Determination for TiCl<sub>4</sub>-Capped MgCl<sub>2</sub> Nanoplate of Heterogeneous Ziegler-Natta Catalyst, ACS Catalysis, 2019, 9, 2599-2609.

### Equipment

Andrew+ Pipetting robot

Multipurpose parallel reactor (developed in-house) Microwave synthesizer with a robotic arm Catalyst screening instruments (developed in-house) Photocatalyst screening instrument (developed in-house) Operando chemiluminescence analyzer (developed in-house) Chemiluminescence imaging instruments (developed in-house) In-situ mid/far-IR spectrometer Laser Raman spectrometer Microplate reader X-ray diffractometer with an autosampler

X-Ray fluorescence spectrometer with an autosampler etc.

### **Teaching policy**

### [Website] URL: https://www.jaist.ac.jp/ms/labs/taniike/en/

There is no core time in our laboratory: The throughput of experiments and the research itself is maximized in order to assure the work-life balance. On the other hand, extensive discussion is regularly made based on experimental group meeting (once a few weeks) and colloquium (once a month). The attendance of domestic and international conferences is fully supported.



### YAMADA-TAKAMURA Lab.

## Professor : YAMADA-TAKAMURA Yukiko <sup>E-mail :</sup> <sub>yukikoyt@jaist.ac.jp</sub>

[Research areas] Materials Science and Engineering, Surface Science [Keywords] nanomaterials, 2D materials, thin films, ultra-high vacuum, hetero-epitaxial growth, surface and interfaces

# Development of nanomaterials based on the understanding of surface and interface



### Skills and background we are looking for in prospective students

We are looking for students who are curious to see how the atoms are aligned at the surfaces and interfaces of materials, and are eager, to understand how these structures determine the properties of materials by carrying out many experiments, calculations, and thinking.

### What you can expect to learn in this laboratory

You are expected to use cutting-edge microscopy and spectroscopy systems without destroying them, and to observe crystal and electronic structures which no one has ever seen. Under such circumstances, you have to be cautious and daring at the same time. Quite often, something goes wrong, and things will not proceed as you planned. You will learn to be patient and flexible to accomplish the original goal, and in the end, you will be able to find something totally new and unexpected. Frequent discussions with faculties and fellow students will make you think logically and critically.

[Job category of graduates] Engineers/researchers in electronics, materials, healthcare, system integrating, machinery industries, and national agencies

### **Research outline**

Modern industry is founded on thin film materials technologies, ranging from protective coatings to electronic devices, and in order to improve their performance, controlling film-substrate interfaces would be critical. The surfaces and interfaces become even more important in the growth of nanomaterials and their properties, since the bulk part is reduced and the surfaces and interfaces become dominant. Our group develops new nanomaterials based on the understanding of surfaces and interfaces obtained by using cutting-edge microscopy and spectroscopy systems and by carrying out first-principles calculations.

One of the main research projects in our group is "silicene", Si-version graphene, and related two-dimensional (2D) materials formed on hetero-epitaxially grown thin films of zirconium diboride (ZrB<sub>2</sub>). ZrB<sub>2</sub> has a very good lattice matching to a wide-gap semiconductor, hexagonal gallium nitride (GaN), and thus, ZrB<sub>2</sub> is a promising buffer layer for GaN growth when it is grown on a low cost, large diameter substrate such as Si wafers.

We discovered silicene, in 2012, while trying to understand the surface structure and properties of diboride thin films grown on Si wafers, thanks to close collaboration with a photoelectron spectroscopy group and first-principles calculation group in JAIST. Our findings attracted lots of interests, and collaborations have expanded to other universities and institutions in Japan and overseas. Through such international collaboration, we have recently succeeded in encapsulating silicene under insulating and inert hexagonal boron nitride monolayer which is another interesting 2D material.

We combine many different material characterization techniques, including those carried out at synchrotron radiation facilities, and also perform first-principles calculations to tackle with unique and novel 2D materials. Recently, we have discovered that, on the surface of  $ZrB_2$  thin film grown on Ge substrate, 2D Ge layer crystallizes into a structure which we predict to have a "flat band" in its electronic structure.

Even in a material studied by many researchers for a very long time, a big surprise

is hidden, which is waiting for you to be discovered. Our students have discovered a new polymorph of a typical layered monochalcogenide, gallium selenide (GaSe), by cross-sectional scanning transmission electron microscopy, and studied its stability and electronic structure by first-principles



calculations. You just have to keep your eyes and mind wide open.

We will not limit our research to the above studies. There are numerous surface and interface problems waiting to be solved. We would like to help you find, understand, and solve your own interesting and challenging questions.

### **Key publications**

- First-principles study on the stability and electronic structure of monolayer GaSe with trigonal-antiprismatic structure, H. Nitta, T. Yonezawa, A. Fleurence, Y. Yamada-Takamura, and T. Ozaki, Physical Review B 102, 235407 (2020).
- Emergence of nearly flat bands through a kagome lattice embedded in an epitaxial two-dimensional Ge layer with a bitriangular structure, A. Fleurence, C.-C. Lee, R. Friedlein, Y. Fukaya, S. Yoshimoto, K. Mukai, H. Yamane, N. Kosugi, J. Yoshinobu, T. Ozaki, and Y. Yamada-Takamura, Physical Review B 102, 201102(R) (2020).
- Van der Waals integration of silicene and hexagonal boron nitride, F. B. Wiggers, A. Fleurence, K. Aoyagi, T. Yonezawa, Y. Yamada-Takamura, H. Feng, J. Zhuang, Y. Du, A. Y. Kovalgin and M. P. de Jong, 2D Materials 6, 035001 (2019).

### Equipment

Ultra-high vacuum thin film growth system, ultra-high vacuum scanning probe microscopes, thin film X-ray diffraction, synchrotron radiation facilities, supercomputers.

### **Teaching policy**

### [Website] URL: https://www.jaist.ac.jp/ms/labs/yukikoyt

An originally designed UHV-CVD system with RHEED and a very unique UHVMBE-XPS/UPS-SPM system are installed in MS Building-IV. We welcome those who are interested in carrying out experiments such as film growth and surface/interface analysis with ultimate resolution, and, more important, who are always curious to find out what is really going on.

### Professor : YAMAGUCHI Masayuki <sup>E-mail :</sup> m\_yama@jaist.ac.jp

[Research areas] Material Design Based on Rheological Approach [Keywords] Polymer Rheology, Polymer Processing, Polymer Blends

# Design of High-Performance Polymer Materials by Rheological Approach



Skills and background we are looking for in prospective students

Basic knowledge of polymer science, chemical engineering and physical chemistry

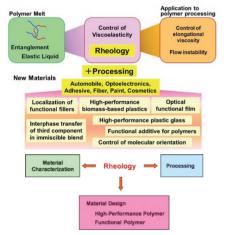
### What you can expect to learn in this laboratory

Students will get the skill to develop a novel polymer material without using polymerization techniques. Basic concepts of polymer processing will be immediately available in industry.

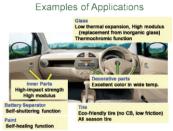
[Job category of graduates] Plastic/Rubber/Fiber Producers; Polymer Processing and Compounding Companies

### **Research outline**

Rheology - the new science of deformation and flow for a material showing complicated mechanical responses - is necessary to develop advanced polymeric materials. Our laboratory is carrying out material design of functional and high-performance polymers based on the rheological approach to create novel displays, next-generation automobile parts, eco-friendly materials including biomass-based plastics, and so on. Moreover, innovation of polymer processing is also studied with our industrial partners, considering trouble-shooting of actual processing operations. Our research activities are outlined below.



1.Rheology provides fundamental information on polymer processing. Based on the experiences and basic information on polymer sciences, extensive study on various processing operations such as foaming, injection-molding and extrusion is performed considering properties of final products. We also continue proposing new ideas to control the rheological properties including elongational viscosity. The obtained results provide new ideas for material design of high-performance or functional polymers. 2.We are carrying out various projects for material design employing conventional and/or newly developed polymers. Novel concepts to improve properties or to provide a specific function are proposed for the application of automobile, electric,



and optical parts. Appropriate molecular structure, molecular aggregation state, and the processing method to obtain the morphology are presented in the field of rubber, fiber, paint, and plastics. Here are the examples of high-performance automobile parts developed by means of rheological modification.

### **Key publications**

- M. Yamaguchi et al., "Modification of rheological responses under elongational flow", in "Polymeric foams; Innovations in technologies and environmentally friendly materials", Ed. S. T. Lee, Chap. 2, CRC, Boca Raton, 2022.
- M. Yamaguchi et al., "Novel methods to control the optical anisotropy of cellulose esters", in "Pulp Production and Processing", Chap. 13, Ed. V. Pope, De Gruyter, Berlin, 2020.
- 3. M. Yamaguchi, "Manufacturing of High Performance Biomass-Based Polyesters by Rheological Approach" in "Handbook of Composite from Renewable Materials", Chap. 2, Eds. V.K. Thakur, M.K. Thakur, Wiley, New York, 2016.

### Equipment

Strain-controlled rheometer; Stress-controlled rheometer, Capillary rheometer; Elongational rheometer, Twin-screw mixer, Dynamic mechanical analyzer; Biaxial stretching machine

### **Teaching policy**

[Website] URL: https://www.jaist.ac.jp/ms/labs/yamaguchi/index-e.html

Our research targets are closed to industrial applications. However, we strongly encourage students to study the basics to propose a novel idea.

### AKABORI Lab.

Associate Professor : AKABORI Masashi <sup>E-mail :</sup> akabori@jaist.ac.jp

[Research areas] Epitaxial growth, Nanostructures, Spintronics [Keywords] Semiconductors, Magnetic metals, Nanofabrication, Electrical measurement, Magnetic field, Low temperature

# Spintronics Research in Semiconductor Nanowires



### Skills and background we are looking for in prospective students

Our laboratory is experimentally studying solid state materials and devices. Therefore, students who like to handle them will be matched with us. The students should better have physics background especially electromagnetism and quantum mechanics, and basic background of solid state physics including semiconductor physics, chemistry, programing, etc. The backgrounds will be helpful for studying in our laboratory.

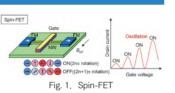
### What you can expect to learn in this laboratory

In our laboratory, the students will operate various equipment. The operation is considered based on principles and logical thinking. Therefore, with understanding and performing the operations, the students will learn the principles and logical thinking way. Also since in experimental studies there are lots of troubles/problems, sometimes it is difficult to obtain expected results and scheduled progress as well. However, by analyzing the troubles/problems and the results with cooperation with other members, the students will pay their own efforts to obtain more good results, and finally will learn problem discovering ability and problem solving ability.

[Job category of graduates] Electronic Devices/Materials, Electrical/Precision Machinery, Communication/Information Technology

### **Research outline**

The information technology supported by the electronics is based on controlling electric charge. The spintronics is controlling not only electric charge but also spin direction for the future information technology. In the IEEE International Road-



map for Devices and Systems (IRDS), the spintronic devices are ranked as important next-generation devices. The most typical spintronic device using a semiconductor (SC) is spin field-effect transistor (spin-FET), which consists of a SC channel having large spin-orbit coupling (InAs, In-GaAs, InSb, InGaSb etc.) and ferromagnetic metal (FM) electrodes (Fig. 1). By using SC nanowire (NW) as the channel, spin relaxation caused by the spin-orbit coupling and elastic scattering is expected to be suppressed in the spin-FET. According to the background, we investigate NW-FM hybrid structures for spintronic applications.

### (1) Formation of SC NW structures

We investigate top-down and bottom-up formation of SC NWs. In the top-down method, we process high-quality SC heterojunctions by using electron beam lithography and etching technique (Fig. 2). In this case, the challenges for coherent spin transport are optimization of the edge shape and suppression of the etching damage. In the bottom-up method, we use molecular beam epitaxy on masked substrates (Fig. 3). In

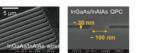


Fig. 2. Wire channel and point contact by top-down methods

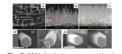
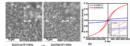


Fig. 3. NWs by bottom-up methods

this case, it is difficult to utilize heterojunctions, however, it is possible to achieve fine shape and size of NWs by optimized growth conditions.

### (2) Formation of SC/FM hybrid structures

We also investigate electrochemical process of SC (ZnO) / FM (Ni or Co) core/shell NW formation (Fig. 4) and molecular beam epitaxial growth of SC (InAs) / FM (MnAs) hybrid structure formation (Fig. 5). In these methods, continuous interface formation between SC and FM is possible. Therefore, it is also expected that spin injection efficiency from FM to SC becomes higher.



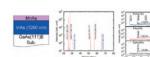


Fig. 4. Electrochemical deposited core/shell NWs

#### (3) Electrical characterization and analysis

We also carry out electrical characterization and analysis of fabricated NW-FM hybrid structures at low temperatures under magnetic fields by using cryostats with superconducting magnets. By non-local resistance

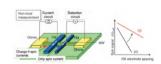


Fig. 5 MnAs/InAs hybrid structure

conducting magnets. By non-local resistance Fig. 6. Non-local measurement measurements under in-plane magnetic fields (Fig. 6), we can obtain the information of spin injection, transport, and detection. Our final aim is the fabrication of spin-FETs which have not

### Key publications

been realized yet in the world.

- S. Komatsu, M. Akabori: "Spin-filter device using Zeeman effect with realistic channel and structure parameters" Jpn. J. Appl. Phys., Vol. 63, pp. 02SP14-1-5 (2024).
- Md. T. Islam, Md. F. Kabir, M. Akabori: "Low-temperature grown MnAs/InAs/MnAs double heterostructure on GaAs (111)B by molecular beam epitaxy" Jpn. J. Appl. Phys., Vol. 63, pp. 01SP40-1-5 (2024).
- K. Teramoto, R. Horiguchi, W. Dai, Y. Adachi, M. Akabori, S. Hara: "Tailoring Magnetic Domains and Magnetization Switching in CoFe Nanolayer Patterns with Their Thickness and Aspect Ratio on GaAs (001) Substrate" Physica Status Solidi B, Vol. 259, pp. 2100519-1-9 (2022).
- D. Q. Tran, Md. E. Islam, K. Higashimine, M. Akabori: "Self-catalyst growth and characterization of wurtzite GaAs/InAs core/shell nanowires" J. Crystal Growth, Vol. 564, pp. 126126-1-7 (2021).

### Equipment

Common-use deposition system (Molecular Beam Epitaxy, Atomic Layer Deposition, Evaporation, Sputter), Commonuse fabrication system (Electron Beam Lithography, Gas Field Ion Source Focus Ion Beam, Reactive Ion Etching), Common-use measurement system (Device Analyzer, Hall Effect Measurement System, Magnetic Property Measurement System) Electrochemical deposition system, Lock-in measurement system, Super conducting magnet system

### **Teaching policy**

### [Website] URL: https://www.jaist-akabori-lab.com/

In our laboratory, we carry out experimental study from formation to characterization/analysis of materials/devices using various equipment. The students are divided into teams by topics, and are asked to have daily team meeting. The staffs join weekly laboratory meeting to grow up communication/presentation/judging skill. Also in the meeting, reading a book and/or paper is carried out to grow up basic scholastic ability and to increase professional knowledge on solid state physics.

AN Lab.

Associate Professor : AN Toshu <sup>E-mail :</sup> toshuan@jaist.ac.jp

[Research areas] nano spin science, spintronics, nano MRI [Keywords] quantum sensing, diamond NV center, magnetic resonance imaging, spin waves, scanning probe microscopy, laser confocal microscopy

# Quantum spin dynamics; sensing, control, and imaging

### Skills and background we are looking for in prospective students

Basic knowledge of physics, condensed matter physics, and electrical engineering. Diligence to master a skill, and will to challenge to new things.

### What you can expect to learn in this laboratory

The objective of this laboratory is detection, control and imaging of spin dynamics at nanoscale. Spin physics such as magnetic resonance, and spin current based on quantum mechanics are explored, in ferromagnetic, antiferromagnetic, and paramagnetic materials, at nanoscale. For nanoscale spin sensing, nitrogen vacancy (NV) center in diamond is used, and combined with confocal microscope and atomic force microscope. Technical skills of electrical engineering for microwaves, optics, and scanning probe microscope are developed.

[Job category of graduates] Manufacturing, analyzing, and development and research work of electronics and materials related companies

### **Research outline**

We focus on study of sensing "spin dynamics" in magnetic materials and its control at nanoscale. We explore novel phenomena related to spin dynamics and extract fundamental physics behind for the application to the spin device and the magnetic sensor device. For this purpose, highly sensitive and high-resolution spatial magnetic sensing and imaging methods are developed (Fig. 1).

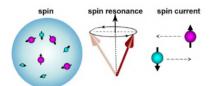


Fig. 1, Spins in electron and nuclei, spin resonance and spin current

#### (1) Nanoscale magnetic field sensing using nitrogen-vacancy center in diamond

Recently, nitrogen vacancy center (NV center) in diamond crystal is attracting much attention for utilizing it as a spin sensor (Fig. 2), since spin state existing in a combination of a carbon defect and nitrogen indiamond named as nitrogen-vacancy center (NV center) was demonstrated to be detected through fluorescence measurement (Gruber and Wrachtup, *et al.*, Science, **276**, 2012 (1997)).

Interestingly, this optically detected magnetic resonance (ODMR) can be used for sensing spins existing around (Fig. 3). Especially, making a NV center as a scanning spin imaging probe (Fig. 4).

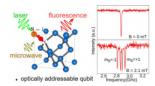


Fig. 2, NV center in diamond, and its magnetic resonance signal

### (2) Long-distance excitation of NV center via surface spin waves

We succeeded to excite NV center by spin waves; collective emotion of spins excited from 3.6 millimeter distance [1]. This will be new system to study interactions of spins.

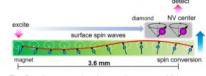


Fig. 3, spin conversion from spin wave to NV center

#### (3) Development of scanning NV center spin sensing probe

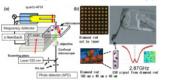


Fig. 4, scanning NV center spin sensing probe combined with AFM

### Key publications

- Yuta Kainuma, Kunitaka Hayashi, Chiyaka Tachioka, Mayumi Ito, Toshiharu Makino, Norikazu Mizuochi, and Toshu An "Scanning diamond NV center magnetometer probe fabricated by laser cutting and focused ion beam milling" Journal of Applied Physics 130, 243903 (2021)
- Dwi Prananto, Yuta Kainuma, Kunitaka Hayashi, Norikazu Mizuochi, Ken-ichi Uchida, and Toshu An "Probing Thermal Magnon Current Mediated by Coherent Magnon via Nitrogen-Vacancy Centers in Diamond" Phys. Rev. Applied 16, 064058 (2021).
- D. Kikuchi, D. Prananto, K. Hayashi, A. Laraoui, N. Mizuochi, M. Hatano, E. Saitoh, Y. Kim, C. A. Meriles, T. An, Long-distance excitation of nitrogen-vacancy centers in diamond via surface spin waves, Applied Physics Express, 10, 103004 1-4 (2017)

### Equipment

Home-made diamond NV center-based spin sensing apparatus, based on confocal microscopy, and atomic force microscopy.

### **Teaching policy**

#### [Website] URL : https://www.an-laboratory.com/english-home/

In our laboratory, spin dynamics is studied, to apply the obtained new insights to "spintroncs" and "nano magnetic resonance imaging" (nano-MRI) fields. Development of unique and ultra-sensitive, and high-resolution experimental system will be performed. For this purpose, it requires a deep knowledge of material science, freewheeling thinking, and ability to solve problem, and we will have a mutual discussion every day to develop skills of each person.

### HAMADA Lab.

Associate Professor : HAMADA Tsutomu E-mail : t-hamada@jaist.ac.jp

[Research areas] Soft matter, Membrane biophysics [Keywords] Soft matter, Artificial cell, Biological membrane, Liposome, Phase separation, Molecular robotics

# Dynamics of artificial cell membranes

### Skills and background we are looking for in prospective students

Basic skills of biochemical experiments, and interest in artificial cell membranes.

### What you can expect to learn in this laboratory

- 1.Experimental skills of artificial cell membranes
- 2. Physical chemistry of soft matter
- 3.Operation of optical microscopes
- 4.Reading and understanding of scientific journals

### [Job category of graduates] Post-doc, Chemicals, Machinery

### **Research outline**

Living cells are a form of self-assembled soft matter. Lipid bilayer membranes are essential components of living organisms. We i) construct artificial lipid vesicles which produce cellular dynamics, such as endocytosis and autophagy, and ii) elucidate the association of biological and nonbiological nano-materials on membrane surfaces.

#### 1. Photo manipulation

We develop a novel system for photocontrol of dynamics of lipid vesicles through the use of a photosensitive molecule. We achieved membrane dynamics: i) triggering of lateral phase segregation, ii) budding vesicular transformation, iii) pore opening through the stabilization of bilayer edge, and iv) membrane fusion. The study could lead to a better understanding of the mechanism of membrane dynamics in living cells and may also see wider applications, such as in drug delivery and biomimetic material design.

#### 2. Interaction with colloids

We investigate the lateral localization and dynamical motion of nano/microparticles within a membrane interface. We found that lateral heterogeneity in the membrane mediates the partitioning of nano/microparticles in a size-dependent manner. The dependence of particle diffusion on the association state was also revealed. The study may lead to a better understanding of the basic mechanisms that underlie the association of nanomaterials within a cell surface.

#### 3. Mechanical response

We study a systematic analysis of lateral phase separation under membrane tension. We applied osmotic pressure directed toward the outside of vesicles to induce membrane tension. Microscopic observations clarified the shifts in phase structures within bilayer membranes with change in tension and temperature. We found that membrane tension can induce phase separation in homogeneous membranes. The study may provide insight into the biophysics of bilayer phase organization under tension, which is an intrinsic mechanical property of membranes.

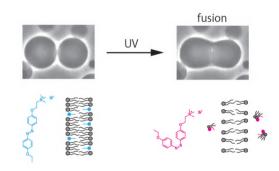


Figure: Photo-induced fusion of lipid vesicles. (Langmuir 2017)

### **Key publications**

- 1. "Photo-induced fusion of lipid bilayer membranes" Y. Suzuki, et al., Langmuir, 33, 2671 (2017).
- "Size-dependent partitioning of nano/micro-particles mediated by membrane lateral heterogeneity" T. Hamada, et al., J. Am. Chem. Soc., 134, 13990 (2012).
- 3. "Domain dynamics of phase-separated lipid membranes under shear flow" T. Hamada et al., Soft Matter, 18, 9069 (2022).

### Equipment

Laser scanning microscope Optical microscope

### **Teaching policy**

[Website] URL: https://www.jaist.ac.jp/ms/labs/hamada/english.html

We aim to find novel phenomena of lipid vesicles to explore new possibilities of the membrane. Through research activities, we would like you to acquire skills with which you can solve a problem by using basic knowledge, and to experience pleasure of learning a thing with curiosity.

### HIRATSUKA Lab.

Associate Professor : HIRATSUKA Yuichi <sup>E-mail :</sup> vhira@iaist.ac.ip

[Research areas] Protein engineering, Mechanical engineering, Nano-biotechnology, Biophysics [Keywords] Molecular robotics, bioMEMS, Molecular motors, Genetical engineering

# Micro-Mechanical Devices Powered by Motor Proteins

Skills and background we are looking for in prospective students

Basic knowledge of biochemistry, biology and protein science or mechanical engineering, and broad intellectual curiosity.

### What you can expect to learn in this laboratory

- \* Protein engineering and skill of genetic engineering
- \* Micro-fabrication (photo-lithography, soft-lithography, etc.)
- \* Protein preparation and biochemical analysis
- \* Operation of optical microscopes
- \* Development of simple software for microscope and other devices

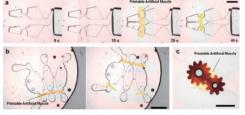
[Job category of graduates] Manufacturer in chemical, mechanical or IT company, etc.

### **Research outline**

Living organisms have developed diverse functions through evolution over a long period of time. Some functions are related to mobility, including muscle contraction, bacteria's swimming and cell division. Nanometer proteins called motor proteins are integrated into motion assemblies with dimensions ranging from the micrometer-scale (bacteria) to the meter-scale (muscle). A motor protein is a molecular machine that converts chemical energy into dynamic force with great efficiency. This is an excellent property that conventional artificial motors do not have. In our laboratory, we are developing biohybrid micro-mechanical devices integrating protein engineering and micro-fabrication technology.

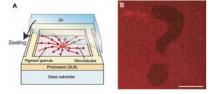
### 1) Printable artificial muscle built from motor proteins

We are developing printable artificial muscle which can be induced the hierarchical self-assembly of motor proteins into an artificial muscle by spatially selected illumination, that can be integrated into engineered systems. The artificial muscle opens the possibility of 3D printing of micro/soft robot built from protein molecules.



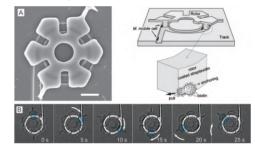
### 2) Optical device driven by motor proteins

We developed an optical device driven by motor protein, which mimicking a molecular system of fish pigment cell, melanophore.



### 3) Micro-rotary motor powered by bacteria or motor proteins

We also developed micro-rotary motor driven by living bacterial or motor proteins. This ATP or glucose-driven rotary motor has a unique feature compared with conventional electronical motors.



### Key publications

- Takahiro Nitta, Yingzhe Wang, Zhao Du, Keisuke Morishima & Yuichi Hiratsuka A printable active network actuator built from an engineered biomolecular motor *Nature Materials* 20, 1149–1155 (2021)
- 2. Susumu Aoyama, Masahiko Shimoike, and Yuichi Hiratsuka Self-organized optical device driven by motor proteins *Proc. Nati. Acad. Sci.* (*PNAS*) 110, 16408-16413 (2013).
- Y. Hiratsuka, M. Miyata, T. Tada and T. Q.P. Uyeda, Micro-rotary motor powered by bacteria, *Proc. Nati. Acad. Sci.* (*PNAS*) 103, 13618-13623 (2006).

### Equipment

Photo-lithography and microfabrication devices, Leaser lithography equipment Protein purification and analysis devices Fluorescence microscope Fermentor, etc.

### **Teaching policy**

### [Website] URL: http://www.jaist.ac.jp/ms/labs/hiratsuka/

We are challenging to develop a novel bio-hybrid micro-mechanical device integrating protein engineering and micro mechanical engineering. To achieve this, we encourage students to get a broad knowledge and flexible ideas and enjoy the research.





### JI Lab.

Associate Professor : JI Yonghoon  $_{ji-y@jaist.ac.jp}^{\text{E-mail}\,:}$ 

[Research areas] Robotics, sensor data processing [Keywords] Mobile robot, robot vision, environmental sensing, SLAM (simultaneous localization and mapping)

# Pioneering Technology for Intelligent Environmental Sensing Using Unmanned Mobile Robot



### Skills and background we are looking for in prospective students

To have basic knowledge of mathematics such as linear algebra and probability theory, and the general concepts of robotics, instrumentation engineering, and machine learning would be desirable. Highly motivated students with curiosity are welcome. In order to implement ideas on robotic systems, it is advantageous if students are accustomed to creating simple hardware and programming languages, especially C<sup>++</sup> or Python.

### What you can expect to learn in this laboratory

Robotics is a special field in which various areas such as mechanical, electronic, computer, control, and instrumentation engineering are seamlessly integrated. Thus, SI (system integration) technology is very important. Depending on the specific research theme, students will be able to acquire a wide range of engineering knowledge. In addition, since we are actively conducting research that is applicable to real sites, students can learn the ability to apply state-of-the-art technology to various problems in our society.

[Job category of graduates] Manufacturing industry, IT industry, academia, etc.

### **Research outline**

We conduct various research required for real-world applications through robot technology. Specifically, we analyze data from the various sensors mounted on the unmanned mobile robot and extract shape information or physical properties distributed in the environment such as material information to utilize them to solve various problems in our society.

### 1. Semantic Map Building by Exploration Robot in Disaster Area

We develop a semi-autonomous mobile robot system that builds a wide-area survey map including semantic information to carry out damage monitoring in disaster areas. To this end, sensor fusion technology is developed for multiple types of sensors mounted on the ro-

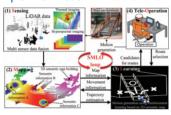


Fig.1 SMLO loop-based survey map building.

bot to build map information including various physical properties of the environment. Each elemental technology as shown in Fig. 1 is developed in cooperation with other universities. The semantic survey map can be used for the prevention of secondary disasters and recovery plans.

#### 2. Underwater Sensing Using Acoustic Camera

Recently, as shown in Fig. 2, the development of acoustic cameras, which can generate high-resolution images in 3D space, even in turbid water, has facilitated our understanding of underwater situations. This

type of sonar sensors is relatively small and can easily be mounted on an underwater robot. Moreover, it can analyze the properties of the material distributed in the environment based on measured data. This

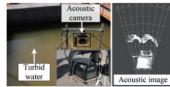


Fig.2 Underwater imaging using acoustic camera.

research focuses on generating a 3D material distribution map using the acoustic camera under a waterfront development environment where human cannot directly access, such as construction and reclamation projects related to airports, ports, and submarine tunnels, etc. Providing the underwater map information to the relevant decision-making organizations, it is expected to be utilized for the future plan of the waterfront development.

### 3. Autonomous Mobile Robot Navigation

Navigation technology for autonomous mobile robots has been intensively studied in recent decades, and many technologies have already been put into practical use. Our goal is to improve the navigation performance of autonomous mobile robots based on measurement data from various next-generation sensors.

### Key publications

- Y. Wang, Y. Ji, H. Woo, Y. Tamura, H. Tsuchiya, A. Yamashita, and H. Asama, "Acoustic Camera-based Pose Graph SLAM for Dense 3-D Mapping in Underwater Environments," IEEE Journal of Oceanic Engineering, 46(3), PP. 829-847, 2021.
- Y. Ji, Y. Tanaka, Y. Tamura, M. Kimura, A. Umemura, Y. Kaneshima, H. Murakami, A. Yamashita, and H. Asama, "Adaptive Motion Planning Based on Vehicle Characteristics and Regulations for Off-Road UGVs," IEEE Transection on Industrial Informatics, 15(1), pp. 599-611, 2019.
- Y. Ji, A. Yamashita, and H. Asama, "Automatic Calibration of Camera Sensor Network Based on 3D Texture Map Information," Robotics and Autonomous Systems, 87(1), pp. 313-328, 2017.

### Equipment

Wheeled and crawler type mobile robots

Sensors for environmental measurement, such as LiDAR, range sensor, optical camera, thermography, acoustic camera, etc.

### **Teaching policy**

#### [Website] URL: http://robotics.jaist.ac.jp/

We aim to cultivate human resources who can contribute to society through robot technology. To this end, it is important to understand the requirement in our society and relevant technological trends. Therefore, we are carrying out research topics applicable to real sites. Next, all students are encouraged to make presentations at domestic and international conferences and write journal papers. Finally, students will improve the following abilities: teamwork, communication, presentation skills through regular meetings in our laboratory as well as collaboration with other universities and companies.

### NISHIMURA Lab.

Associate Professor : NISHIMURA Shun <sup>E-mail :</sup> s\_nishim@jaist.ac.jp

[Research areas] Catalyst chemistry, Solid catalyst, Alloy catalyst, Biomass transformation [Keywords] New energy sources, Metal nanoparticle, Solid acid/base catalyst, Catalyst design, Mechanistic study

# Development of new solid catalyst process Challenge the issues on energy & resources!



### Skills and background we are looking for in prospective students

Basic calculation skill, Careful data processing capacity, and Safety consciousness are necessary for participation. Some experiences on Physical chemistry, Organic chemistry, Inorganic chemistry, Analytic chemistry and/or Catalyst chemistry would be a great help for your studying. We welcome your aggressive curiosity and inquiring minds.

### What you can expect to learn in this laboratory

Development of new solid catalyst process is constructed with a variety steps: Catalyst design  $\rightarrow$  Catalyst preparation & Conditioning  $\rightarrow$  Performance evaluation & Conditioning  $\rightarrow$  Characterizations (Kinetics, XRD, TEM-EDS, N<sub>2</sub> ads/des, FT-IR, UV-vis, Raman, XPS, XAFS etc)  $\rightarrow$  Modeling/Hypothesis  $\rightarrow$  Verification  $\rightarrow$  Scope. Moreover, there is more than one crucial factor on the target catalysis. Accordingly, following the step to reveal the role of catalyst, the student would learn the various analytical methods and skills to combine the many aspects of data.

[Job category of graduates] Chemical and material suppliers in the area of car, plastic, polymers and surfactant manufactures.

### **Research outline**

Catalyst technology has been a key role on manufacturing in our life. Thus, development of highly-functional catalytic process would lead drastic impacts on our society towards more green and sustainable styles. For instance, the development of catalytic ammonia ( $NH_3$ ) generation from nitrogen ( $N_2$ ) in air process had opened a lot of new avenues to supply *N*-incorporating compounds. In particular, after this achievement, chemical fertilizer and dynamite manufacturings were contributed to the growth of population and facilitation of industrial technology [Noble Prize for Chemistry in 1918].

The targets of our laboratory are i) new catalyst design on the basis of conventional transformation skills on fossil resources, and ii) construction of biomass-based utilization process over solid catalyst, in order to fabricate a low carbon society.

### [Metal-supported catalyst: New design and Mechanistic studies]

The catalytic performance of metal-supported catalyst; *i.e.* active metal centers supported on inorganic/organic solid surface, was attributed to i) electronic state and shape of the active metal center, ii) environment around the active metal center, and iii) properties of support. Studying on the relationships among these factors by using fine/uniform as-prepared metal-supported catalysts reveals the crucial factors for the target reaction. In previous our reports, we found the highly-reactive alloy-supported catalysts [ex. CS&T 2013, ACS Catal 2013, CheSusChem 2015, ACS sustainable Chem Eng 2019], the organic-linkage assisted metal-supported catalysis [ex. JPCC 2014, Asian JOC 2017] and the specific support designs for high reactivity or stability [ex. J. Mater. Chem. A 2014, Catal Lett 2021].

### [Development of solid catalyst assisted biomass transformations]

On the basis of the carbon neutral concept, the biomass utilization is a one of important approaches to fabricate sustainable society. However, low life-cycle assessment (LCA) is an issue for this transformation. To accelerate the green technology, development of highly-efficient catalytic transformation process has been investigating. In previous our reports, we proposed the bio-fuel production process with an atmospheric hydrogen gas [Catal. Today 2014], the production of highly value-added chemicals from inedible biomass resource [ex. ChemSusChem 2013, ACS Omega 2018, Catal Commun 2019, Catalysts 2019], and the highly-active acid-base catalyzed processes [ex. BCSJ 2012, ChemSusChem 2014, CS&T 2016].

### **Key publications**

- S. D. Le, S. Nishimura: Selective hydrogenation of succinic acid to gamma-butyrolactone with PVP-capped CuPd catalysts. Catal. Sci. Technol. 12 (2022) 1060.
- K. Anjali, S. Nishimura: Efficient Conversion of Furfural to Succinic Acid using Cobalt-Porphyrin based Catalysts and Molecular Oxygen. J. Catal. 428 (2023) 115182
- X. Li, S. Nishimura: Synthesis of 5-Hydroxymethy-2-furfurylamine via Reductive Amination of 5-Hydroxymethyl-2-furaldehyde with Supported Ni-Co Bimetallic catalysts. Catal. Lett. 154 (2024) 237.

### Equipment

Evaluation of catalyst performance: GC, HPLC, GC-TOFMS, FTICR-MS, NMR for liquid, etc Characterization of catalyst: XRD, Gas Adsorption/desorption, SEM/TEM, XPS, NMR for solid, FT-IR, TPR/TPD, pulse method, etc

For a specific elucidation methods: Out-side institutes (ex. KEK-PF, SPring-8) for in-situ/ex-situ XAFS analysis.

### **Teaching policy**

#### [Website] URL : https://www.jaist.ac.jp/~s\_nishim/index.html

Labo meeting for introduction of previous papers and/or discussion of recent data is held in one time per two weeks. Core-time is not determined, however, the students have to pay attentions to their healthy/regular life in the labo. Presentations in domestic/international conference are recommended.

We hope more than one paper/proceeding reports would be published according to your achievement for all members.

### OKEYOSHI Lab.

Associate Professor : OKEYOSHI Kosuke <sup>E-mail :</sup> okeyoshi@jaist.ac.jp

[Research areas] polymer chemistry, photochemistry, soft matter [Keywords] polymeric gels, water, geometry of soft materials, photofunctional materials, energy conversion

# Polymeric organization inspired from natural environment and biomaterials



### Skills and background we are looking for in prospective students

We are seeking individuals who have experience or fundamental knowledge about polymer science, physical chemistry, material science, photochemistry, and soft matter. In particular, individuals who can handle challenges, and are innately curious and persevering are encouraged to apply.

### What you can expect to learn in this laboratory

Academic subjects: Polymer science, photochemistry, soft matter science, colloidal science, surface chemistry, geometry, and non-linear science. Additional skills: Logical thinking and understanding, experiment designing, scientific verification, high-quality presentations, ability to communicate in English.

[Job category of graduates] Manufacture of materials, healthcare industry, etc.

### **Research outline**

Many beautiful patterns are visible in nature. For example, living organisms are created via self-organization from small molecules. This is derived not only from the material, but is also the result of strong environmental influence. In fact, life has evolved to adapt to changing environments, resulting in diverse spatial patterns and rhythms.

Furthermore, studies aimed at creating patterns by regulating the physical environment using artificially synthesized molecules have been performed in antiquity. However, synthetic molecules are seldom compatible with medical or industrial applications, and may not coexist in natural environments. In contrast, in our latest study, we demonstrated that natural polysaccharides can reconstruct hierarchical patterns from water. Hence, when we understand "how" and "why" patterns appear, we can acquire novel material designs that can fulfill the criteria of biocompatibility and environmental adaptability.

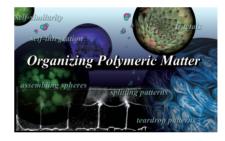
### 1. DRY & WET: Self-organization of natural polysaccharides

We are investigating the mechanism via which polysaccharides reproduce geometric patterns in centimeter scale in vitro. In particular, by controlling physicochemical conditions, we are exploring the law of spatial recognition exhibited in polysaccharides under dry environment. In a non-equilibrium environment, macromolecules are organized in both micro and macro forms. The fact that actual living organisms survive in dry environments while maintaining their body moisture could be critical for understanding biopolymer evolution.

### 2. Pattern control of soft materials

Regardless of their origin (biological or synthetic), several types of soft materials can be morphologically controlled by stress at the materials' interface. Only small environmental differences, such as slight changes in mechanical energy, can change shapes and patterns, *e.g.*, spatial/temporal self-similarity. These patterns can be used in medicine as novel biomimetic materials that can efficiently adapt to the external environment.

Based on these viewpoints, the ultimate goal is to determine the laws regulating these phenomena and natural beauty. In summary, we are investigating one of the biggest enigmas of natural science, i.e., why does life create patterns?



### Key publications

- 1. DRY & WET: meniscus splitting from a mixture of polysaccharides and water. Okeyoshi K, Polymer Journal 52, 1185 (2020).
- Vapor-sensitive materials from polysaccharide fibers with self-assembling twisted microstructures. Budpud K, Okeyoshi K, Okajima MK, Kaneko T, Small 16, 2001993 (2020).
- Polymeric design for electron transfer in photo induced hydrogen generation through a coil-globule transition. Okeyoshi K, Yoshida R, Angewandte Chemie International Edition 58, 7304 (2019).

### Equipment

Optical microscopes, optical spectrometer, polarized light devices, image analysis devices, fluorescence measurement instruments, viscometer, densimeter, dynamic light scattering, electron microscopes, etc.

### **Teaching policy**

#### [Website] https://sites.google.com/oke-acgroup.com/web

During the training period prior to working in society, we will support the selected candidate to expand his/her potentials to the best of our capacity. Our group provides a diverse environment both in terms of research and culture. This is a priceless opportunity for constructing a versatile scientific personality. Based on the above-mentioned research objectives, the candidate will consciously pursue research on the following lines: 1.Develop the abilities of logical thinking and foresight.

2.Design and verify hypotheses through experiments and discussions

3.Learn to use scientific language for public outreach purposes.

### SHINOHARA Lab.

Associate Professor: SHINOHARA Ken-ichi E-mail : shinoken@jaist.ac.jp

[Research areas] Polymer Chemistry, Artificial-Life Function [Keywords] Nanomachine, Polymer Synthesis, AFM Video

# Direct Observation of Single Molecule of a Polymer Molecular Machine Driven by Thermal Fluctuations



### Skills and background we are looking for in prospective students

Basic knowledge of organic chemistry and polymer chemistry is necessary for research on functional polymer synthesis. Also, in single molecule imaging research to analyze the structure and dynamics of single polymer chain, understanding of the mechanism of microscope equipment is required.

### What you can expect to learn in this laboratory

The objective of our laboratory is to create novel nanomachine such as a molecular motor by a chiral helical  $\pi$ -conjugated polymer in an organic media at room temperature. The members of this laboratory learn basic knowledge and technique of organic/polymer synthesis, single-molecule imaging, computer simulation (all-atom MD), and design of molecular machines.

[Job category of graduates] Chemical companies, Electronics companies, Food-related companies, Public officials (teachers)

### **Research outline**

### Single-Molecule Imaging of a Polymer

Direct observation of a polymer chain deepens the understanding about its structure and function. The study of single polymer chains was made possible after the scanning probe microscope (SPM) and the total internal reflection fluorescent microscope (TIRFM) had been developed. Our group succeeded in the direct observation of the long-chain branch (LCB) structure in a low density polyethylene (LDPE), and the structural dynamics of a polymer chain in a functionalized styrene-butadiene rubber (SBR) and an ethylene-propylene (EP) rubber measured by a fast-scanning atomic force microscope (FS-AFM). Single-molecule imaging of a macromolecular motion in a chiral helical polymer was achieved by the FS-AFM, and the diffusion coefficient of each part of the polymer chain was measured. On the other hand, the photonic function of the light emission from a rigid-rod conjugated polymer was measured using TIRFM at room temperature. The light-emission from a single polymer chain as it slowly and dynamically changes over a cycle lasting a few seconds has been successfully detected using TIRFM with a built-in spectroscope.

### A Polymer Molecular Motor

If a molecule can move unideirectionally using thermal fluctuation, a molecular motor having the function of substance transport and morphological change is created. In our recent study, molecular walking along a rail of a synthetic helical polymer (*Scheme 1*) was discovered by AFM video imaging. This walk was unidirectional processive movement in an organic solvent at room temperature (*Fig.1*).

This result is a breakthrough as the first step in order to create an artificial life-function as a synthetic molecular motor driven by a thermal fluctuation in non-aqueous media.

Scheme 1. Synthetic Route of a Chiral Helical Polymer

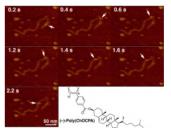


Fig. 1. Single Molecular Unidirectional Processive Movement along a Helical Polymer Chain in a Non-aqueous Media

### Key publications

- K. Shinohara, S. Yasuda, G. Kato, M. Fujita, H. Shigekawa: Direct observation of the chiral quaternary structure in a π-conjugated polymer at room temperature, *J. Am. Chem.* Soc. **123**, 3619-3620 (2001); Editors' Choice, *Science* **292**, 15 (2001).
- K. Shinohara, Y. Makida, T. Oohashi, and R. Hori: Single-Molecule Unidirectional Processive Movement along a Helical Polymer Chain in Non-aqueous Medium, *Langmuir*, 38 (40), 12173-12178 (2022).
- K. Cheng, K. Shinohara, O. Notoya, M. Teraguchi, T. Kaneko, T. Aoki Synthesis and Direct Observation of Molecules of 2D Polymers: With High Molecular Weights, Large Areas, Small Micropores, Solubility, Membrane Forming Ability, and High Oxygen Permselectivity, Small, 202308050 (2023).

### Equipment

Fast-Scanning Atomic Force Microscope (FS-AFM), Scanning Tunneling Microscope (STM), Total Internal Reflection Fluorescence Microscope (TIRFM), NMR, Super Computer System for all-atom MD Simulation of a Polymer Chain in Solvent, Analytical System of Single-Molecular Motion of a Polymer

### **Teaching policy**

### [Website] URL: https://www.jaist.ac.jp/ms/labs/shinohara/

In the SHINOHARA laboratory, we instruct students to conduct research themes as their own, rather than passively studying. Specifically, the supervisor will actively communicate with students, voluntarily perform experiments according to the student's abilities, and develop the ability to find and solve the scientific problems themselves. By repeating these processes, students are able to answer important questions such as what is scientific research, which in turn leads to awareness as future excellent researchers and engineers.

### TSUTSUI Lab.

Associate Professor : TSUTSUI Hidekazu E-mail : tsutsui@jaist.ac.jp

[Research areas] biophysics, neurophysiology, molecular & cell biology, bioengineering [Keywords] neuron, synapse, molecular sensor, next generation electrophysiology, bio-imaging

# Molecular sensors & devices for interfacing with electrical activities in live cells.



### Skills and background we are looking for in prospective students

Background knowledge in brain science, molecular and cell biology, biophysics and/or electrical engineering may help to smoothly lunch a solid research project. However, we support students with limited prior knowledge in the related subjects. We rather give a high importance to scientific motivations and intellectual curiosity.

### What you can expect to learn in this laboratory

Basic and advanced experimental techniques concerning molecular biology, electrophysiology, fluorescence imaging, and bio-engineering; Comprehensive understanding of principles underlying various cellular phenomena and their applications to biomedical science.

[Job category of graduates] Research and development in biomedical industry, manufacture, information technology

### **Research outline**

We seek to develop molecular sensors and devices that permit precise spatiotemporal detections of dynamic functions in live cells. Our main focus is given to parallel measurements of cellular electrical activities.

Cellular electrical signal occurs as a voltage difference across cell membrane and rapidly propagates, playing essential roles in a variety of physiological functions. Those include secretion, contraction and neural transmission. In particular, dynamic modulation of the flow of electrical signals in the neuron networks is thought to underlie the neural function. In seeking to reveal its fundamental principles, one of the most awaited techniques is the sensitive detection of spatiotemporal electrical activity in a complex network of excitable cells.

One on-going approach is a protein-based voltage probe that can be genetically encoded under the control of cell-type specific promoters. We investigate biophysical properties of membrane proteins that undergo voltage dependent structural transitions and feedback the knowledge to the design of robust voltage probes. We are also interested in visualizing electrical phenomena in organelle membrane as well as biomedical applications of the sensor technologies including the development of an efficient drug screen platform. Techniques used in this topic are the conventional molecular biology, electrophysiology, photometry, and fluorescence imaging.

By taking an advantage of the advanced facilities in the JAIST nanomaterial and technology center, we have launched a new project: innovative micro-fabrication based electrophysiology combined with organic electronics. Techniques used in this topic are micro-fabrications, electrical engineering, as well as molecular biology.

Apart from these topics, we pursuit various curiosity-driven researches, mainly focusing on fluoresce proteins. For example, we have developed a variant of coral fluorescent protein that forms diffraction-quality crystals within mammalian cells. This expression system allowed the direct determination of its crystal structure as

well as observation of the crystallization process and cellular responses. We are trying to reveal general mechanism underlying intracellular protein crystallizations. We also focus on interactions of fluoresce proteins with metal thin film and particles, and their potential applications to cell biology.

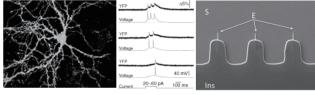


Figure 1

(left) A hippocampal neuron expressing a fluorescence sensor for membrane voltage.

(center) Simultaneous photometry and electrophysiological recordings. (right) A SEM image of the prototype device for parallel interfacing of cells.

### Key publications

- 1. Farha et al., Interface-specific mode of protonation-deprotonation reactions underlies the cathodic modulation of fluorescence protein emission. Appl. Phys. Express 13 (2020).
- Farha et al., Electric-field control of fluorescence protein emissions at the metal-solution interface. Appl. Phys. Express 12 (2019).
- Tsutsui, H. et al., Improved detection of electrical activity with a voltage probe based on a voltage-sensing phosphatase. J. Physiol., 591, 4427- 4437 (2013).

### Equipment

fluorescence/luminescence live cell imaging systems electrophysiology and photometry rigs electrochemical analyzer cell/tissue culture & molecular biology equipment Sputtering system; SEM (JAIST common facilities)

### **Teaching policy**

### [Website] https://www.jaist.ac.jp/ms/labs/tsutsui/wordpress/

Although research is basically driven by intellectual curiosity, the requisites are comprehensive understanding of related background, learning reliable experimental procedures as well as the ability to logically evaluate the observation. These will be emphasized in the early stage of laboratory work. Lab activities include a biweekly progress report presentation and journal club. Students are also encouraged to read through a specified textbook to learn the related subjects and scientific culture.

## UEDA Lab.

Associate Professor: UEDA, Jumpei <sup>E-mail :</sup>

[Research areas] Solid State Chemistry, Photochemistry [Keywords] Phosphor, Storage Phosphor, White-LED, Optical thermometer, Optical Pressure Sensor

# Development of Optically Functionalized Materials Based on Electronic Structure and Local Coordination



### Skills and background we are looking for in prospective students

Motivation to improve yourself and to progress a research topic, to open a new scientific area through studying actively with your curiosity and discussing with other researchers is necessary. We respect your research background.

### What you can expect to learn in this laboratory

Our research topic includes material preparation, physical property evaluation and application study. You will acquire research planning, reorganization of issues and logical thinking as basic capability, and wide knowledge and various technical skills in solid state chemistry and photochemistry. Presentation skills also can be obtained through several research meetings.

Specific skills: Material preparation (powder, ceramics, transparent ceramics, glass, single crystal of inorganic compounds), Physical property evaluation (XRD, XAS, basic optical measurements, luminescence lifetime, photoconductivity, VUV spectroscopy, measurements for storage phosphors, high pressure measurement)

[Job category of graduates] Chemical and material suppliers, manufactures of electric devices

### **Research outline**

There are many luminescent materials and devices around us such as white LED lighting, laser projectors, TV and smartphone displays. These luminescent devices include inorganic phosphors with luminescence center (rare earth and transition metal ions). The optical properties of the phosphors vary greatly depending on the type of luminescence center, its geometrical and chemical coordination environment, and the electronic structure of the host material. Our research group investigate the factors to determine the optical properties and design new optical functional materials.

### Generation of while light!

White LEDs and laser-excited white light sources consist of blue LED (or laser) and visible phosphors. Recently, green and red phosphors with a narrow luminescence band width for display application and non-quenching phosphors by high power laser excitation are studied. Through the elucidation of physical phenomena, we strategically create phosphors with higher properties.



Control of luminescence properties by changing geometrical and chemical environments

### Storage of light energy!

Persistent phosphors can show contentious luminescence even after stopping excitation source. We design persistent phosphors by controlling the photoinduced electron transfer process based on the electronic structures of inorganic compound with luminescence ions.

### Sensor using luminescence!

The luminescence properties vary by temperature and pressure. Thus, the phosphors can be used as optical thermometers and pressure sensors.



persistent phosphor

### • Other research topics

Photochromism, luminescence quenching, Mechano-luminescence, pressure induced phase transition

### Key publications

- 1. Jumpei Ueda, Bull. Chem. Soc. Jpn. 94, 2807(2021)
- 2. Jumpei Ueda, Setsuhisa Tanabe, Opt. Mater. X 1, 100018 (2019)
- 3. Jumpei Ueda et al. J. Phys. Chem. C 119, 25003 (2015)

### Equipment

Vacuum Gas Replacement Furnace, XRD, Fluorescence spectrophotometer, Cryostat Wavelength tunable OPO laser, Optical measurement system for storage phosphors, Diamond anvil cell

### **Teaching policy**

Our research group holds research meeting and journal club (introduction of state-of-the-art research) once a week, which can be adjusted depending on the number of laboratory members. Core-time is 9 am to 5 pm. The research topic includes material preparation, physical property evaluation and application. Thus, you learn wide knowledge and various technical skills in solid state chemistry and photochemistry. Basically, all of laboratory members need to give a presentation in a domestic or international conference. We also recommend publishing the research results to an international journal as a first author or co-author.

## YAMAGUCHI Takumi Lab.

### Associate Professor : YAMAGUCHI Takumi E-mail : takumi@jaist.ac.jp

[Research areas] Biomolecular science, Biofunctional chemistry, Biophysical chemistry, Organic chemistry, Supramolecular chemistry [Keywords] Carbohydrate, Molecular recognition

# Sweet Science: Analytical and applicative research of bio-functional sugars



### Skills and background we are looking for in prospective students

Our research interests are in analyses of biomolecules, mainly carbohydrates, and creation of bio-inspired functional molecules. Although having basic knowledge of organic and biological chemistry as well as physicochemical background is preferable, the high motivation for challenging and developing the new research field is primarily valued. We welcome students of drive!

### What you can expect to learn in this laboratory

Study of carbohydrates has been attracting considerable attention as a next task in various fields including drug development and medical research. You address the task by learning and employing multidisciplinary knowledge and skills as in synthetic organic chemistry, analytical chemistry and biotechnology. You will also improve the ability to promote projects based on creative ideas and logical thinking.

### [Job category of graduates] Chemical and material industry

### **Research outline**

### 1. Analysis of biomolecules

Carbohydrates play crucial roles in a variety of biological events such as cell-cell communications. For example, many of proteins in the living system are decorated with carbohydrate moieties, which mediate molecular recognition processes. In addition, recent evidence has demonstrated that carbohydrates on cell membranes are targets for various proteins that are associated with serious diseases, e.g., Alzheimer's disease and Guillain-Barré syndrome. Our research seeks the underlying molecular basis for the function of carbohydrates, providing knowledge for the rational design of drugs and biomolecular engineering that contribute towards a detailed understanding of living systems.

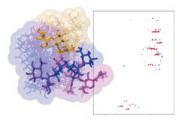


Fig 1. We have developed a methodology to describe the dynamic structure of oligosaccharides based on NMR techniques in conjunction with molecular dynamics simulations.

### 2. Creation of bio-inspired molecules

Using the combination approaches based on the chemical design and hybridization of artificial molecules with biological materials can generate unique molecular systems having the fundamental functions of life. Toward controlling biological functions of oligosaccharides and expanding in their applications, we attempt to create artificial glycomolecules (neoglycoconjugates) through bridging between synthetic chemistry and biomolecular science. The effective hybrid approaches have been enabling not only the establishment of dynamic systems mimicking nature and thus well-defined models for biophysical understanding, but also the creation of those with highly advanced, integrated functions.

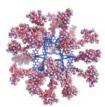


Fig 2. Attachment of oligosaccharides to a spherical supramolecule provided neoglycoclusers, which possess potential functional ability through multivalent interactions.

### Key publications

- Delineating the dynamic conformations of oligosaccharides by combining molecular simulation and NMR spectroscopy, T. Yamaguchi, *Trends Glycosci. Glycotechnol.* 32, E93–E98, 2020.
- Comprehensive characterization of oligosaccharide conformational ensembles with conformer classification by free-energy landscape via reproductive kernel Hilbert space, T. Watanabe, H. Yagi, S. Yanaka, T. Yamaguchi, K. Kato, *Phys. Chem. Chem. Phys.*, 23, 9753–9760, 2021.
- Experimental and computational characterization of dynamic biomolecular interaction systems involving glycolipid glycans, K. Kato, T. Yamaguchi, M. Yagi-Utsumi, *Glycoconj. J.* 39, 219–228, 2022.

### Equipment

NMR spectrometer Mass spectrometer Computer cluster Liquid chromatography system

### **Teaching policy**

#### [Website] URL: https://www.jaist.ac.jp/ms/labs/t-yamaguchi/index.html

To design, create and utilize your own molecules is emphasized. We also aim to improve communication skills through research activities, such as scientific discussions with colleagues in the lab and presentations of research results at academic conferences.

### YAMAMOTO Lab.

### Associate Professor : YAMAMOTO Yuko S. E-mail : yamayu@jaist.ac.jp

[Research areas] surface enhanced spectroscopy, quantum optics, catalysts [Keywords] Spectroscopy, Raman spectroscopy, surface enhanced spectroscopy, surfaceenhanced Raman scattering (SERS), tip-enhanced Raman scattering, nanomaterials

# Exploring the nanoworld using surface enhanced spectroscopy



### Skills and background we are looking for in prospective students

"I love research activity!" "I enjoy scientific experiments!" "I love creating new materials!" "I want to improve the world with my great discovery!" At least one of these should apply to you because such motivations are essential for starting researches in our lab. I teach you the knowledge necessary to make achievements and the method of learning new techniques. Students with grand ambitions are particularly welcome.

### What you can expect to learn in this laboratory

The ability to open new horizons through your own efforts. This skill is of use in many areas of our life, but there are few opportunities to learn it. I recommend you to have several skills in our lab: (1) sensitively perceive the present situation to forge your own path to new possibilities, (2) an appropriate awareness of the present issues and possess the solving skills of these issues, (3) a high level of linguistic ability, including presentation skills, communication skills, and written composition skills, (4) strong interpersonal skills to obtain funding and build consensus. I support you as you learn these through advancing your research. I also support you in studying abroad or starting a venture business during or after your time in our laboratory.

[Job category of graduates] Chemistry manufacturers, start-ups, etc.

### **Research outline**

What actually happens in the world at a nanometer scale? We explore the "nanoworld" using surface-enhanced spectroscopy. Generally speaking, spectroscopy makes us possible to obtain the chemical composition of measuring targets with irradiating the laser light or other light sources and careful analysis of the absorption, reflection and scattering of light. Surface-enhanced spectroscopy is a technique of dramatically increasing the intensity of the absorption, reflection and scattering of light using the surface of nanostructures which composed of free electron-rich metals such as silver or gold. This phenomenon enables us to measure the chemical composition of measuring targets at a very small scale – nanometer-order.

In our lab, we constructed an original surface-enhanced spectroscopic system which enable to measure even single molecule, so we believe there are great expectations from the aspects of both research and industrial applications.

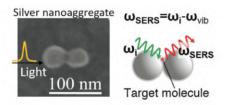


Figure. Schematic of surface-enhanced Raman scattering measurement.

Based on "surface-enhanced Raman spectroscopy", one of the surface-enhancement spectroscopy, we can obtain the information on the vibration level of molecules.

Our lab promotes both fundamental researches and applied researches. Current research topics of us are as follows:

### 1.Surface analysis of catalytic chemical reactions using surface-enhanced Raman scattering

In recent years, nanostructures made of coinage metals such as gold and silver, showing strong plasmon resonance in the visible light region are considered very promising as next-generation heterogeneous photocatalyst materials. A conventional heterogeneous photocatalysts such as titanium dioxide (TiO<sub>2</sub>), which is well-known for its Honda-Fujishima effect, requires ultraviolet light to produce the catalytic effect. Meanwhile, chemical reactions such as water splitting( $2H_2O \rightarrow 2H_2 + O_2$ ) and dissociation of hydrogen molecules ( $H_2 \rightarrow H^+ + H^+$ ), which had

conventionally been considered to require the energy of ultraviolet light, have been realized with the visible light using a new heterogeneous photocatalyst discovered in the early 2010s, and this research is progressing globally to investigate the new phenomenon of such heterogeneous photocatalysts.

In our lab, we focus on the photochemical reactions which occur on a surface of metal nanoparticles with plasmon resonance, monitored by surface-enhanced Raman scattering with irradiation of visible light.

### 2.Looking ahead to surface-enhanced Raman scattering

About 50 years have passed since the surface-enhanced Raman scattering effect was discovered in the 1970s. Although the mechanism of the surface-enhanced Raman scattering phenomena is becoming increasingly deeply understood, there are mysteries that still remain. Our lab focuses on these mysteries and explores the most advanced areas of surface-enhanced Raman scattering. At the same time, we are working to discover new physical or chemical phenomena that emerge from surface-enhanced Raman scattering and understand their mechanisms.

If you would like to see references or papers on research results, please feel free to email to Yamamoto (yamayu@jaist.ac.jp) or visit Yamamoto's office. I will give you copies of our papers.

### **Key publications**

- Judith Langer, Yuko S. Yamamoto et al, "Present and Future of Surface Enhanced Raman Scattering", ACS Nano, 14, 28-117, 2020.
- Yuko S. Yamamoto\*, Yuya Kayano, Yukihiro Ozaki et al, "Single-Molecule Surface-Enhanced Raman Scattering Spectrum of Non-Resonant Aromatic Amine Showing Raman Forbidden Bands", arXiv:1610.08270, 2016.
- Yuko S. Yamamoto\*, Tamitake Itoh\*, "Why and how do the shapes of surface-enhanced Raman scattering spectra change? Recent progress from mechanistic studies", J. Raman Spectrosc., 47, 78-88, 2016.

### Equipment

Surface-enhanced Raman microscope (homemade) Density functional theory (DFT) calculation system

### **Teaching policy**

#### [Website] URL : (under construction)

I have personally studied what kind of environment is suitable for the basic research. As a result, I found that a free and unfettered research environment is the best for effective basic research. Therefore, our laboratory basically does not have a core time. Information exchanges with members in our lab and confirmation of progress with peers are conducted in the weekly general meeting and seminars. I encourage students to come our lab who can autonomously manage their own research activities properly. I recommend all the students in our lab to make presentations in domestic/international conferences about once a year to express our research results to the world. To the best of my skills, research themes of students are established taking into consideration the range and direction of each students' interests and according to their preferences, with consideration of the research theme presented by me. Basically, we aim to publish our research results in the international journals. Of course, I always provide individual guidance for each students as needed. Students are encouraged to actively make use of my knowledge and experiences.

# MURATA Lab.

Senior Lecturer : EGUCHI Keitaro

E-mail : eguchi@jaist.ac.jp

[Research Areas] Surface Physical Chemistry, Organic electronics [Keywords] Organic thin film, Operando measurement, Organic memory device, nanotechnology



# Master the Surface and Interface: Pioneering Future-Oriented Organic Semiconductor Devices

### Skills and Background we are looking for in Prospective Students

Students who have majored in chemistry or physics or who have worked with vacuum equipment will find it easier to engage in research. However, as the saying goes, "What one likes, one will do well." If you engage in research that interests you, you will quickly acquire specialized knowledge and skills.

### What you can expect to learn in this laboratory

Students will be able to learn the basic concepts of molecular science and solid state physics through research on organic thin films. In addition, through experiments, students will understand the principles of operation of experimental equipment and experimental techniques, and students will learn how to operate them correctly and how to acquire and interpret experimental data correctly. Also, students can improve their technical writing skills, which are necessary for writing scientific papers and reports, and their presentation skills, which are necessary for academic presentations.

### [Job Category of Graduates]

Semiconductor industry, electronics industry, Chemical company

### Research Outline

"The interface is the device." is a phrase attributed to Nobel Prize winner in physics Herbert Kroemer. The interface between various materials can be a device with new functions. At the surfaces and interfaces where the environment is different from that of the bulk, new properties of materials that were hidden in the bulk properties may emerge. Our research field is such surfaces and interfaces. We are addressing the creation of functional devices that operate with new mechanisms by precisely designing interfacial materials, interfacial structures, and interfacial electronic states and the development of methods for measuring electronic states under device operating conditions.

■ Development of functional organic semiconductor devices We are developing devices with memory functionality by combining organic semiconductors and ionic liquids. We are trying to control the memory characteristics in 2-terminal devices and 3-terminal field-effect transistors.

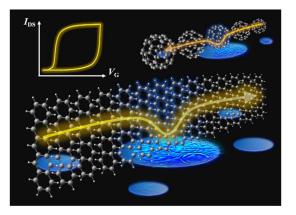


Figure. Schematic diagram of the interaction between electric currents flowing through organic semiconductors and ionic liquids.

Elucidation of the electronic structure of organic thin films under device operation conditions

We are developing measurement methods under the device operating environment to evaluate the structure and electronic states of molecular materials in electronic devices under operation. We will deepen our understanding of how electric currents flow through organic thin films by "observing" states that cannot be "observed" in general measurements. We will also clarify how the state of electrons in the inactive and active states of devices is related to device properties, leading to the improvement of device properties and the development of new devices.

### **Key Publications**

- 1. Keitaro Eguchi and Hideyuki Murata, "Evolution of the Ionization energy in Two- and Three-Dimensional Thin Films of Pentacene Grown on Silicon Oxide Surfaces", The Journal of Physical Chemistry Letters 12, 9407-9412 (2021).
- 2. Keitaro Eguchi and Hideyuki Murata, "Electronic States of Pentacene Thin Films at Interfaces with Ionic-Liquid Layers Probed by Photoelectron Yield Spectroscopy", The Journal of Physical Chemistry C 127, 14940-14948 (2023).
- Keitaro Eguchi and Hideyuki Murata, "The ionization energy of αsexithiophene and p-sexiphenyl in 2D and 3D thin films grown on silicon oxide surfaces", Physical Chemistry Chemical Physics 26, 8687-8694 (2024).

### Equipment

Ultra-high vacuum system / high-vacuum system, photoelectron yield spectrometer / Inverse photoelectron spectrometer / X-ray photoelectron spectrometer, atomic force microscope, X-ray diffraction meter, electrometer, UV-VIS-NIR spectrometer

### Teaching Policy

[Website] URL : https://www.jaist.ac.jp/ms/labs/murata/en/index.html

We will decide on the student's research theme with the student based on the student's interests. We will teach you how to conduct experiments, so please brush up and improve your skills through daily experiments and enjoy your experiments. As research events in our laboratory, we have a paper introduction and a research meeting once a month respectively to discuss the contents. We will give you guidance so that you can present your research at conferences and publish it as a paper in a scientific journal.

### TAKAMURA Lab.

Senior Lecturer : HIROSE Daisuke <sup>E-mail :</sup> d-hirose@jaist.ac.jp

[Research areas] Functional oxides, biosensors, liquid processes [Keywords] MOD method, thin-filmtransistor, biomolecule detection, biochip. printed electronics

# Creation of highly functional materials from liquids for visualization of biology and the environment



### Skills and background we are looking for in prospective students

Curiosity, the challenge of research, and the will to enjoy unexplained and unknown phenomena. No special knowledge is required, as we will guide you from the basic level of knowledge. We welcome students from any field.

### What you can expect to learn in this laboratory

In our research, we will be conducting experiments in a variety of fields. Through research, you learn research perspectives and ideas that are not bound by your field of study. You obtain the ability to solve problems through logical thinking and task-performance skills. Through presentations at conferences and seminars, you will be able to acquire the ability to make presentations and communicate effectively.

[Job category of graduates] Semiconductor manufacturing equipment maker, Electronic component companies, Measuring equipment companies

### **Research outline**

We are creating products based on the metalorganic decomposition (MOD) method. his method is a technique to produce oxides with various electrical properties. Furthermore, we have discovered that oxides and intermediates fabricated by this MOD method have specific characteristics. Our research and development of new sensing devices and patterning methods are based on the combination of these features and semiconductor processes.

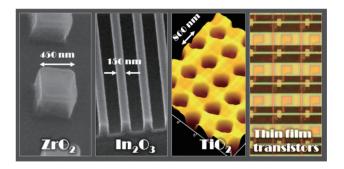
### Highly sensitive oxide sensing devices

We have been researching and developing oxide thin-film transistor-type nucleic acid sensors that enable rapid and sensitive measurement.



### **Oxide Mold Formation Technology**

We have developed a low-energy, low-cost direct printing method for oxides using nanoimprinting. This technique enables easy fabrication of sub-micron scale patterns.



### Key publications

- Submicron titania pattern fabrication via thermal nanoimprint printing and Microstructural analysis of printable titania gels, D.Hirose, H. Yamada, T. Jochi, K. Ohara and Y. Takamura, *Ceramics International*, online, (2024)
- Rapid and Highly Sensitive Detection of Leishmania by Combining Recombinase Polymerase Amplification and Solution-Processed Oxide Thin-Film Transistor Technology, W. Wu, M. Biyani, D. Hirose and Y. Takamura, Biosensors, vol. 13, 8, p. 765, (2023).
- 3. Origin of the thermal plasticity property of zirconium oxide gels for use in direct thermal nanoimprinting, D. Hirose, J. Li, Y.Murakami, S. Kohara and T. Shimoda, Ceramics International, vol.44, p. 17602, (2018).

### Equipment

Electronic device fabrication equipment (photolithography, sputtering,nanoimprinting), electrical characteristics evaluation equipment (semiconductor parameter analyzer, impedance analyzer), shape evaluation equipment (SEM, AFM), material properties evaluation equipment (TG-DTA, FT-IR, UV-vis, XRD, XPS, contact angle meter)

### **Teaching policy**

Our laboratory aims to visualize biology and the environment based on MOD technology to produce functional oxides from liquids. We are targeting all kinds of molecules around us and applying them to society and our daily lives. We are now at a stage of great growth. Let's combine your ideas with our technology to create new visualization sensors! In our research, we will set a theme in line with your interests. We will support you to clear your subjects one by one toward your goal.

### MAENOSONO Lab.

E

[Research Areas] [Keywords] E-mail : mari@jaist.ac.jp Nanomaterials; Cell biology

Nanoparticles; Bioapplications



### Nanobiotechnology

### Skills and Background we are looking for in Prospective Students

Students who have a strong sense of curiosity, like making an effort and have ambitions to improve are suitable to join our lab. Taking the initiative regarding your research is very important. Communication skills and a spirit of cooperation are also important since we often do collaborations.

Senior Lecturer : TAKAHASHI Mari

### What you can expect to learn in this laboratory

General knowledge regarding: synthesis, characterization and analysis of nanoparticles; the characteristic features found in metal, magnetic and semiconductor nanoparticles; cell biology. The spirit to boldly tackle new projects.

### [Job Category of Graduates]

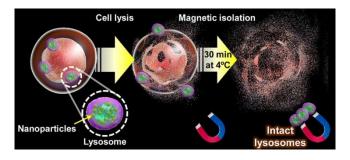
Industry and academic research institutes

### Research Outline

Bioapplications of nanoparticles (NPs) are attracting more attention every year. We utilize the characteristic features of NPs, which are different to those of bulk materials, for a variety of applications, though we mainly focus on the following three areas. In each case, everyone experiences the entire flow from synthesis and characterization to application.

### 1. Isolation of cellular organelles using magnetic NPs

The comparison of proteins in certain organelles between normal cells and cells which have functional deficiencies is important in order to clarify the molecular mechanisms of diseases. To isolate cellular organelles, we perform magnetic separation using magnetic NPs. Magnetic NPs are synthesized, and their surfaces are modified with biomolecules. Then, the NPs are introduced to cells and the magnetic separation of organelles is performed followed by biochemical analysis. This research will contribute to new drug discovery and development.



### 2. Immunoassay using magnetic particle spectroscopy

In order to keep healthy and have a long life, the improvement of the accuracy and efficiency of early stage disease detection technology becomes more and more important. Magnetic particle spectroscopy (MPS) has the potential to become a new immunoassay technique. We prepare different types of magnetic NPs and evaluate the NPs with MPS to create probes which are highly sensitive. Our final goal is to establish a multi-analyte MPS-based immunoassay system.

### 3.Optogenetics using upconversion NPs

Upconversion NPs can convert long-wavelength incident light to short-wavelength emitted light. In Optogenetics, cells with genetically-introduced photoreceptors are used to manipulate cellular activity by light stimulation. Using upconversion NPs and near infrared light, which has high biopermeability, we try to control cellular activity.

### **Key Publications**

- D Maemura, T S Le, M Takahashi, K Matsumura, and S Maenosono: "Optogenetic Calcium Ion Influx in Myoblasts and Myotubes by Near-Infrared Light Using Upconversion Nanoparticles" ACS Appl. Mater. Interfaces 15 (2023) 42196
- 2.T S Le, M Takahashi, N Isozumi, A Miyazato, Y Hiratsuka, K Matsumura, T Taguchi, S Maenosono: "Quick and Mild Isolation of Intact Lysosomes Using Magnetic–Plasmonic Hybrid Nanoparticles" ACS Nano 16 (2022) 885
- 3.T S Le, S He, M Takahashi, Y Enomoto, Y Matsumura, and S Maenosono: "Enhancing the Sensitivity of Lateral Flow Immunoassay by Magnetic Enrichment Using Multifunctional Nanocomposite Probes" Langmuir 37 (2021) 6566

### Equipment

Transmission electron microscope (TEM); Scanning TEM (STEM); Xray diffractometer (XRD); X-ray photoelectron spectroscopy (XPS); Nuclear magnetic resonance (NMR); Superconducting quantum interference device (SQUID); Dynamic light scattering (DLS); Ultraviolet–visible spectroscopy (UV-Vis); Confocal laser scanning microscope (CLSM) etc.

### Teaching Policy [Website] URL : https://www.jaist.ac.jp/~shinya/index-en.html

We always launch new projects and thus there are a lot of things to investigate through both experiment and literature review. We expect that students spontaneously think about what to do next instead of waiting for instructions from professors. To achieve this, we will support you and cultivate your knowledge when considering your future plan. Please talk to us freely whenever you have concerns about or want to discuss your research thoroughly.

Japan Advanced Institute of Science and Technology School of Materials Science