3-2. IROAST International Joint Research Travel Support Program

No.	Name	Destinations Period
3-2-1	**Hamid HOSANO** IINa	Imperial College London, UK August 15, 2023 – August 28, 2023
3-2-2	**Kei ISHIDA** CWMD	Middle East Technical University, Türkiye September 2, 2023 – September 16, 2023
3-2-3	**Kwangsik KWAK** FAST	Karlsruhe Institute of Technology, Germany August 20, 2023 – September 18, 2023
3-2-4	**Ruda LEE** IINa	Korea Basic Science Institute (KBSI), Korea August 18, 2023 – August 31, 2023
3-2-5	**Ruda LEE** IINa	Sungkyunkwan University, Korea December 24, 2023 – January 24, 2024
3-2-6	**Yasuyuki MORITA** FAST	Zhejiang University, China December 12, 2023 – December 16, 2023
3-2-7	**Yuta NAKASHIMA** FAST	National University of Singapore, Singapore November 25, 2023 – November 28, 2023
3-2-8	**Shin-Ichi OHIRA** FAST	1) Mahidol University, Thailand 2) Universitas Islam Indonesia, Indonesia January 25, 2024 – January 31, 2024
3-2-9	**Reetu Rani** IROAST	1) Chulalongkorn University, Thailand 2) Suranaree University of Technology, Thailand February 18, 2024 – February 25, 2024

3-2-10	**Mitsuru SASAKI** IINA	1) Hall at the Hotel Sant Boi, Barcelona, Spain 2) University of Valladorid, Valladorid, Spain	
		September 9, 2023 – September 16, 2023	
3-2-11	**Yoshihiro SEKINE** POIE	The 12th International Symposium on Nano & Supramolecular Chemistry (ISNSC-12)	
		July 21, 2023 – July 27, 2023	
3-2-12	**Kohei SHIMAMURA** FAST	University of Southern California, USA	
		December 26, 2023 – January 8, 2024	

FAST：Faculty of Advanced Science and Technology

IINa：Institute of Industrial Nanomaterials

CWMD：Center for Water Cycle, Marine Environment and Disaster Management

POIE：Priority Organization for Innovation and Excellence

3-2-1	Keratin Nanoparticle Aggregation: Experimental and Population Balance Evaluations		
Name	Hamid HOSANO	Title	Professor
Affiliation	Institute of Industrial Nanomaterials Email: hamid@kumamoto-u.ac.jp		
Period of Travel	August 15, 2023 – August 28, 2023		
Visited Researcher	Stelios RIGOPOULOS	Title	Reader
Affiliation	Imperial College London, UK		

1. Overview and significance of the international research collaboration

Imperial College London (ICL) is a leading public research university in UK, with 14 Nobel laureates. It is ranked 8 in the Times Higher Education and 6 in QS World University Rankings. The ICL has several world class centers including Department of Brain Sciences, Department of Bioengineering, Centre for Blast Injury Studies, Graphene Study Group (Computational Materials Science), and Nanomaterials (Department of Mechanical Engineering), with research interests related to activities of the IROAST and the Institute of Industrial Nanomaterials (IINa), Kumamoto University.
In this respect collaboration with Prof. Stelios Rigopoulos, Department of Mechanical Engineering, ICL, was proposed to understand the underlying mechanism of protein nanoparticles aggregation and study keratin nanoparticle formation.
Prof. Rigopoulos's research focuses on advanced theoretical and computational methods, including Computational Fluid Dynamics (CFD), population balance modelling, stochastic and machine learning methods for modelling physical and engineering problems, with applications to crystallization, nanoparticle manufacturing and environmental flows.
Collaboration with Prof. Ghajari, ICL, for traumatic brain injuries has also been performed to understand the mechanisms and consider appropriate prevention methods.

2. Research achievements and progress of the international joint research

In a collaborative study with Prof. M-Nejad (IROAST International Internship Program supported the study), we used feather to produce keratin nanoparticles. Feather is the main waste of the chicken slaughterhouses and needs to be managed properly to prevent environmental pollution. The study resulted in synthesizing the smallest reported keratin nanoparticles [Journal of Cleaner Production, 335:130331, 2022, https://doi.org/10.1016/j.jclepro.2021.130331]. This waste managing research has been attracting considerable attention for industrial and medical applications. Low cost, biodegradability, low immunogenicity, and colloidal stability of recycled feather keratin makes it suitable to produce protein-based nanomaterials. To further understand the underlying mechanism of keratin nanoparticles aggregation, we started a joint research with Prof. Rigopoulos. This study would be crucial to develop our medical projects with keratin nanostructures. The visit served to discuss and prepare a joint research manuscript regarding population balance modelling of our new experimental results of keratin protein nanoparticle formation.
During the visit, Trauma Brain Injuries project with Prof. Mazdak Ghajari and Dr. Xiancheng Yu (Dyson School of Design Engineering, ICL) was also discussed and arranged. Hosano has been performing in-vivo animal blast brain injuries experiments in collaboration with Department of Neurosurgery, School of Medicine; Dr. Ghajari and his team are leading experts to perform numerical simulations of brain injuries. We planned collaboration to simulate in-vivo results to

further explain mechanisms of brain damages.

3. Prospect for further research collaboration with the visited university/institution

Discussions and lab visits were performed at Prof. Rigopoulos and Dr. Xiancheng Yu laboratories to facilitate the joint researches and collaborations. Prospects and required experimental devices and simulation facilities in the ICL, and experiments in the IINa, Kumamoto University, were discussed and arranged. The draft of a joint journal research article was prepared, further collaborative programs and further joint articles will be followed up during future visits. We planned to apply for a JSPS Bilateral Joint Research progam and UK-Japan grant to financially support the joint researches.

Meeting with Prof. Rigopoulos and his Ph.D. students at the Department of Mechanical Engineering, Imperial College London.

Discussion after meeting with Prof. Rigopoulos's team.

Meeting with Dr. Xiancheng Yu, Imperial College London.

3-2-2	Application of Deep Learning to various issues in Hydrological Engineering		
Name	Kei ISHIDA	Title	Associate Professor
Affiliation	Center for Water Cycle, Marine Environment, and Disaster Management Email: keiishida@kumamoto-u.ac.jp		
Period of Travel	September 2, 2023 – September 16, 2023		
Visited Researcher	Ali ERCAN	Title	Associate Professor
Affiliation	Middle East Technical University, Türkiye		

[Details of activities]

1. Research outline and its perspective (in approx. 50-80 words and attach 1-2 relevant photographs)

The primary goals of this research consist of three key aspects: employing advanced deep learning approaches to address hydrological problems, evaluating the suitability of such deep learning techniques, and simultaneously developing new deep learning architectures specifically designed for hydrological challenges. In addition, this research endeavor aims to examine the nature of relationships between variables that deep learning algorithms can identify. This research aims to improve the reliability of using deep learning in the field of hydrological engineering.

2. Research progress and results in the fiscal year

In September, I visited the Middle East Technical University, Türkiye to proceed the collaborative research with Dr. Ali Ercan (Figure 1). Initially, discussions were conducted regarding the preparation of the manuscript. During these discussions, a collective agreement was reached that a detailed examination of the ERA5 reanalysis data, frequently employed as input for deep-learning models, is required. Informed by this consensus, the structure and content of the paper will be guided by the insights gleaned from this analysis. Pursuant to this agreement, I collaborated with Dr. Ercan and his student research team to analyze the ERA5 reanalysis data. For instance, we extracted various variables, including precipitation, air temperature, and evapotranspiration. Subsequently, we explored the trends and their inflection points at each grid in the ERA5 dataset, which boasts a spatial resolution of 25 km and an hourly temporal resolution. Notably, the data set has recently been extended to cover the period from 1940, enhancing its utility for global climate change assessments (Figure 2). Our analyses also encompassed trends in drought indices, precipitation indices, and temperature indices. In addition, Those analyses were conducted at multiple scales, including continental, national, and watershed levels (Figure 3). Through these comprehensive analyses, we identified significant shifts in these variables globally, attributable to climate change.

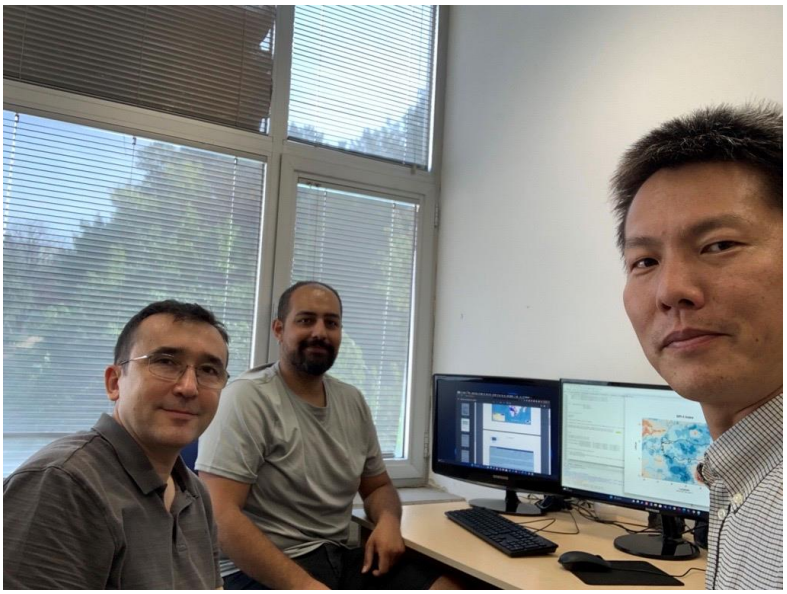


Figure 1 Meeting with Dr. ERCAN and his student

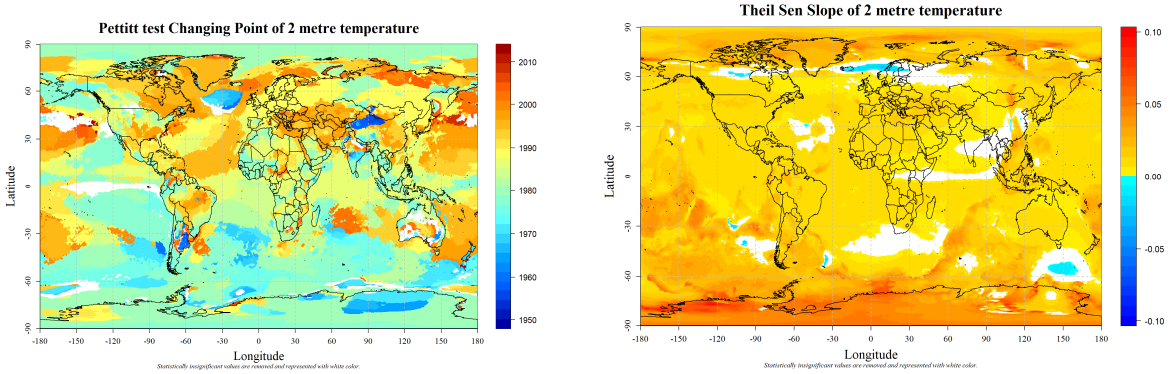


Figure 2 Global-scale climate change analyses

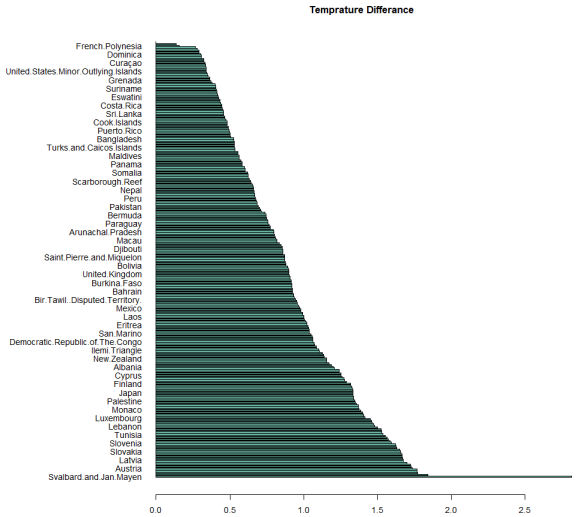


Figure 3 Country-scale climate change analyses

3-2-3	Micromechanical characterisation of microstructures damaged during rolling contact in martensite and austenitic stainless steels		
Name	Kwangsik KWAK	Title	Assistant professor
Affiliation	Faculty of Advanced Science and Technology, Kumamoto University Email: kwak@msre.kumamoto-u.ac.jp		
Period of Travel	August 20, 2023-September 18, 2023		
Visited Researcher	Martin DIENWIEBEL	Title	Professor
Affiliation	Karlsruhe Institute of Technology, Germany		

[Details of activities]

1. Research outline and its perspective. While bearings are one of the most widely used components in industrial machinery, improvement of the resistance to rolling contact fatigue (RCF) is still required to achieve the longer life of bearings. The RCF in bearing steels arises under extreme conditions such as a higher contact pressure or a higher friction rate. Due to the accumulation of RCF, the raceway surface is damaged, leading to crack initiation in the altered microstructure. Therefore, it is essential to understand the correlation between microstructural evolution and corresponding mechanical properties. This study aims to investigate the micromechanical properties of damaged layers on wear tracks created in several loading levels. Friction tests will be performed using a micro-tribometre (Fig.1) at Karlsruhe Institute of Technology (KIT), Germany, and micro-bending tests will be carried out using a micro-bending testing machine (Fig. 2) from Kumamoto University.

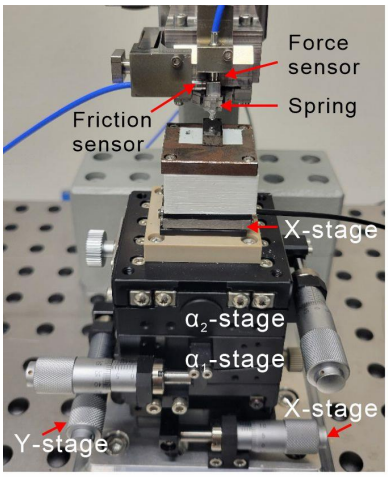


Fig. 1 Micro-tribometre

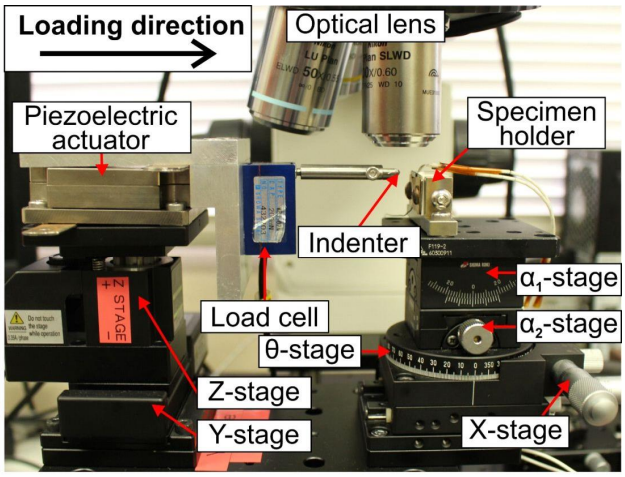


Fig. 2 Micro-bending testing machine

2. Research progress and results in the fiscal year

In FY2023, the friction tests were performed using a micro-tribometre at KIT. The material used in this study was a 100Cr6 bearing steel. In a sphere-on-flat-setup, a 100Cr6 steel sphere with a diameter of 3 mm was used as a countrebody. The sphere was glued onto a double-leaf cantilever with spring constants of kt = 2.781 and kN = 5.034 mN / μm. The micro-friction tests were performed in dry and lubricated contacts at room temperature, an air atmosphere, and normal ambient humidity. Two different normal forces (165 and 402 mN) were loaded, which corresponded to 750 and 1008 MPa of Hertzian contact pressure. 1000 linear reversible cycles were conducted at a stroke length of 2.5 mm and speeds of 1.0 mm s^{-1}.

The normal and friction forces were measured continuously during the tests.

Fig.3 shows the relationship between the mean coefficient of friction (CoF) and the cycle of samples tested at 402 mN in the dry metal–metal contact. While the CoF of samples tested in the dry condition varied, those showed values above approximately 0.3. Meanwhile, in the lubricated contact, the variation of CoF was small and the values indicated almost constant. Fig. 4 depicts the confocal image of the wear track and scanning ion microscope image of the cross-section after focused ion beam machining of the sample (402 mN-d3-1) tested under a normal force of 402 mN. The width of the wear tract was determined to be approximately 170 μm (Fig. 4(a)). The FIB milling was performed to observe the cross-section of the wear tract, as shown in Fig. 4(b). While the cross-section of the sample exhibited martensite microstructure, it was difficult to distinguish the damaged layer.

This year, we succeeded in creating a simulated wear tract using a micro-tribometre, however, the damaged layer was not able to identify. It is necessary to observe local microstructure changes through high magnification analysis using an electron back-scattered diffraction (EBSD) or transmission electron microscopy (TEM).

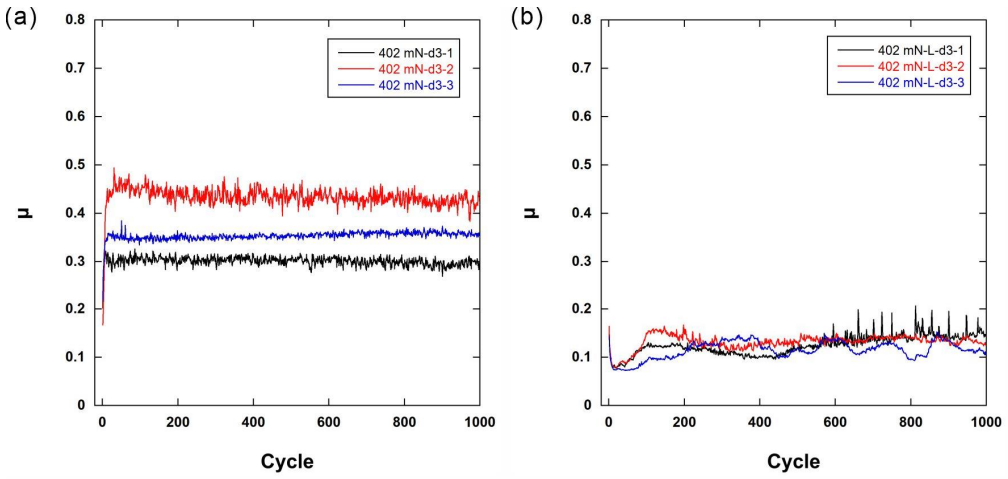


Fig. 3 Friction coefficient versus cycle at 402 mN normal force in (a) the dry metal-metal contact and (b) the lubricated contact.

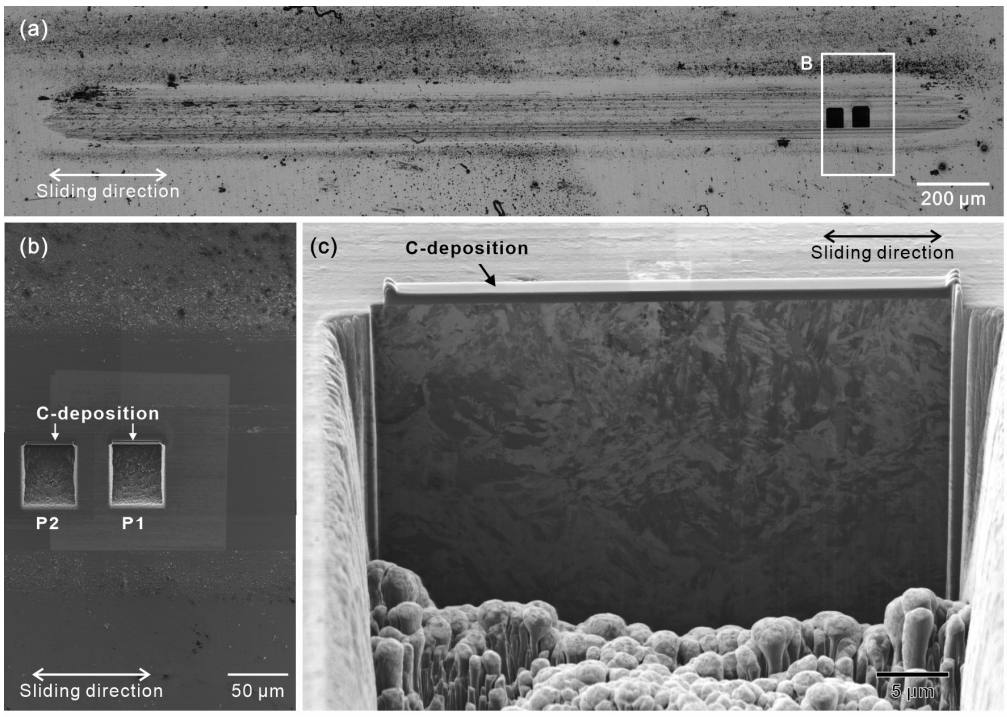


Fig. 4 (a) Confocal image of the wear track of 402 mN-d3-1 sample. (b) Scanning ion microscope image of region B in (a) and (c) high magnification of P2 in (b).

3. Research plan for the next year
   The microstructural morphology of wear tracks will be examined by EBSD or TEM. After microstructural analysis, a micro-bending test is performed using the cantilever specimen containing the RCF damaged layer extracted using FIB. In addition, the micromechanical characterisation of the microstructure with damaged layers introduced by RCF will be extend to stainless steels such as type-304 and type-316 to investigate the effect of phase transformation on their friction properties.

4. List of journal papers (with IROAST as your affiliation) published between April 2023 and March 2024.
   Not Applicable

5. List of awards, grants, and patents
   Not Applicable

3-2-4	Super-resolution integrated real-time imaging of nucleus EGFR and multidrug resistance phenomena in breast cancer		
Name	Ruda LEE	Title	Associate Professor
Affiliation	Institute of Industrial Nanomaterials (IINa) Email: aeju-lee@kumamoto-u.ac.jp		
Period of Travel	August 18, 2023-August 31, 2023		
Visited Researcher	Seung-Hae KWON	Title	Principal Investigator
Affiliation	Korea Basic Science Institute (KBSI, Seoul)		

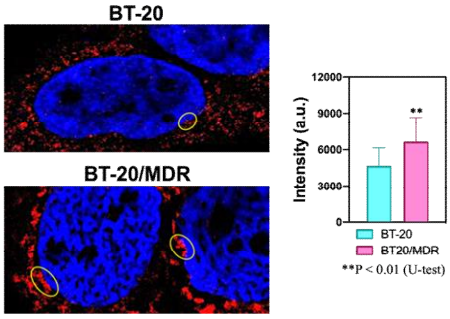
[Details of activities]

1. Research outline and its perspective

A better understanding of the underlying molecular interactions of receptor-multidrug resistance (MDR)-immune cells in a 3D environment is required to develop successful therapeutic strategies to overcome MDR. Live cell imaging of the MDR mechanism is less prone to experimental artifacts and can provide more reliable and relevant information than fixed cell microscopy. This study aims to be the first in the world to systematically understand the drug delivery process by examining interactions among nuclear receptor-MDR-immune cells through real-time imaging.

2. Research progress and results in the fiscal year

Quantification of the nucleus membrane was successfully done. We found the significance of the results and got high-resolution images of the nucleus receptor images. Furthermore, the genomic analysis started to find the reason for receptor translocation after acquiring MDR characteristics.



3. Research plan for the FY2024

Currently, we are focusing on cancer genomics. Data indicate that receptor translocation is related to genome evolution. To concrete the hypothesis, five more TNBC cell lines will be tracked, and the specific receptor-negative cell lines will be examined. These research findings will be discussed with Prof. Hoon KIM at Sungkyunkwan University (SKKU).

3-2-5	Characterization of human Extrachromosomal DNA for overcoming multi-drug resistance		
Name	Ruda LEE	Title	Associate Professor
Affiliation	Institute of Industrial Nanomaterials (IINa) Email: aeju-lee@kumamoto-u.ac.jp		
Period of Travel	December 24, 2023 - January 24, 2024		
Visited Researcher	Hoon KIM	Title	Associate Professor
Affiliation	1) Korea Basic Science Institute 2) Sungkyunkwan University		

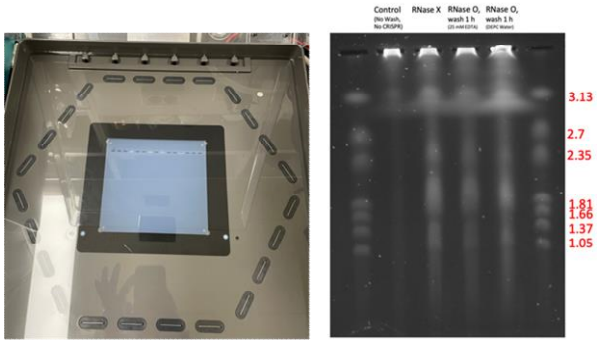
[Details of activities]

1. Research outline and its perspective

Extrachromosomal DNA (ecDNA)-based oncogene amplification frequently occurs in most cancer types and differs from chromosomal amplification. And ecDNA in multiple cancer types leads to poor patient outcomes. Numerous scientific investigations have shown that ecDNA-mediated oncogene amplification contributes to cancer therapy resistance. Thus, we aimed to suggest new insights into the role of ecDNA in drug-resistance cancer.

2. Research progress and results in the fiscal year

The ecDNA extraction conditions were set up with my support, and we succeeded purification of ecDNA from 10 cell lines. The ecDNA extraction was the most important to move smoothly to the next step. Currently, we are starting to organize the drug-resistance cell lines ecDNA copy number analysis by DNAseq and RNAseq.



ecDNA extraction

3. Research plan for the FY2024

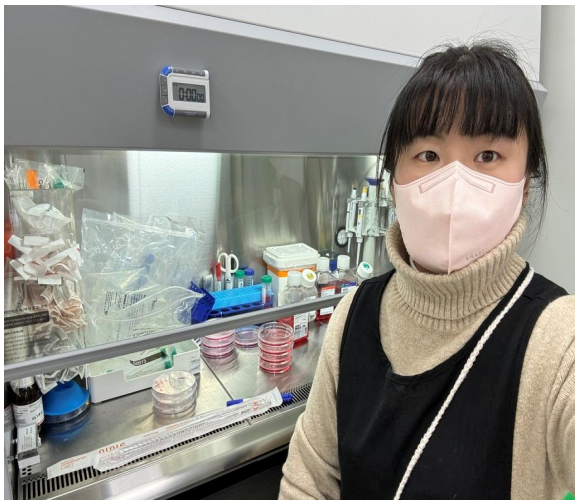
The ecDNA extraction was performed from cell lines. We expect the cDNA extraction to be done in patient-derived primary cells to reflect the cancer environment. Samsung Hospital has already approved the IRB and started gathering the patient samples. The team will be working on investigating the cancer's genomic evolution.

4. List of journal papers

- Antimetabolite Prodrug Delivery for Non-small Cell Lung Cancer. **R Lee**, S Tanigawa, Y.I Park, **H Kim**. *Korean Society for Biotechnology and Bioengineering Journal* 38(4): 236-243 (2023).

5. List of awards, grants, and patents

- Grant apply: FY2023 国際共同研究加速基金（国際共同研究強化）



At Korea Basic Science Institute (KBSI)

At the Multi-University Festival Research Team Meeting

3-2-5	Study on new organelle-targeted nanoparticles for DDS		
Name	Yasuyuki MORITA	Title	Professor
Affiliation	Faculty of Advanced Science and Technology Email: ymorita@kumamoto-u.ac.jp		
Period of Travel	December 13, 2023 - December 16, 2023		
Visited Researcher	Yang JU	Title	Chair Professor
Affiliation	Zhejiang University, China		

[Details of activities]

1. Research outline and its perspective

Outline: This project aims to develop organelle-targeting nanocarriers directed at the subcellular organelle level in order to achieve high-efficiency drug delivery.

Perspective: Delivering drugs to targeted tissues and cells is highly effective in reducing toxicity and improving therapeutic effects. Enhancing this delivery resolution to the level of subcellular organelles means maximizing their efficacy to the limit. In this project, we create DDS nanocarriers by modifying the surface of nanocarriers, which use gold nanoparticles as the core material and are coated with mesoporous silica for carrying drugs, with small molecules that target each organelle.

2. Research progress and result in the fiscal year

The research contents and the results are as follows:

(1) Selection of gold nanoparticles

For hyperthermia and drug diffusion, the size of gold nanoparticles used as a heat source utilizing surface plasmon resonance was selected (see the 2023 Master's thesis of Mr. Keishi Fukumoto), who is my lab's member.

(2) Determination of targeted organelles and selection of modifying small molecules

The purpose of this trip is this topic. And I discussed this matter with Prof. Ju. As the results, the targeted organelle was chosen to be the mitochondria due to the broad scope of application. And as the surface-modifying molecule for targeting, two polyelectrolytes (PSS and PDDAC) were selected.

3. Research plan for the next year

The remaining research contents are as follows:

(3) Coating with mesoporous silica

Mesoporous silica is coated on the surface of the gold nanoparticles for drug loading.

(4) Evaluation of targeting ability and cytotoxicity

We will quantitatively evaluate the targeting performance and cytotoxicity of the fabricated DDS nanocarriers using cells.

4. List of journal papers published between April 2023 and March 2024.

NA

5. List of awards, grants, and patents

Taking advantage of this travel opportunity, I gave a lecture on the topic of “Prologue for establishing tumor mechanics.” Subsequently, a certificate of appreciation was awarded.


荣誉证书
CERTIFICATE OF HONOR
感谢 日本熊本大学 Prof. Yasuyuki MORITA：
莅临浙江大学机械工程学院青年教师发展论坛并作题为“Prologue for establishing tumor mechanics”的特邀报告。
浙江大学机械工程学院
2023年12月15日

3-2-7	Novel Cancer Medical Technology Using Liquid Biopsy		
Name	Yuta NAKASHIMA	Title	Associate Professor
Affiliation	Faculty of Advanced Science and Technology Email: yuta-n@mech.kumamoto-u.ac.jp		
Period of Travel	November 25, 2023- November 28, 2023		
Visited Researcher	Chengkuo LEE	Title	Associate Professor
Affiliation	National University of Singapore, Singapore		

[Details of activities]

This oversea travel was carried out for startup of international joint research. The objective of this international joint research is to develop the bio-sensing technology using MEMS (Micro Electro Mechanical Systems) devices and techniques. I met with Prof. Chengkou Lee of National University of Singapore (NUS), who will conduct the joint research, at an international conference (Transducers 2023 at Kyoto) held in June to discuss the outline of this research cluster. In this oversea travel, I visited NUS and observed on-campus facilities and equipment, as well as equipment and technology owned by Prof. Lee's laboratory. Also, we had discussions facilitated by an on-the-spot question-and-answer session. After the observation, we had discussion including each other's staff and students, discussed the technologies that this research cluster is desired, and discussed how to proceed with international collaborative research in the future. As a result, we agreed to do the international joint research and to achieve the objective. Moreover, it was decided that Ms. Akaike (Ph.D. student, research cluster member, and Torahiko Terada Fellowship student) will study abroad for three months from January to March 2024 to promote this project. In the future, we will promote international joint research and international exchange involving each other's students.

Fig.1 UTown of NUS.

Fig.2 A part of clean room (Campus facility).

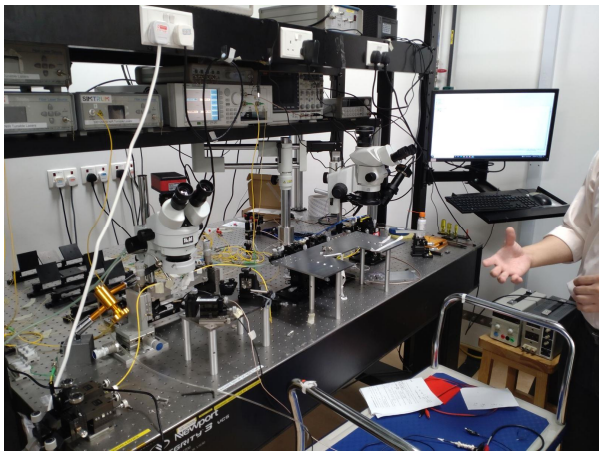


Fig.3 Research equipment (Prof. LEE's lab.).

Fig.4 Prof. Lee, Ms. AKAIKE, and NAKASHIMA (from left side).

3-2-8	Ion extraction with molecularly imprinted membrane and application to nano particle analysis		
Name	Shin-Ichi OHIRA	Title	Professor
Affiliation	Faculty of Advanced Science and Technology International Research Organization for Advanced Science and Technology Email: ohira@kumamoto-u.ac.jp		
Period of Travel	Jan. 25, 2024 – Jan. 31, 2024		
Visited Researcher	Atitaya SIRIPINYANOND	Title	Associate professor
Affiliation	Mahidol University, Thailand		
Visited Researcher	Ganjar FADILLAH	Title	Assistant professor
Affiliation	Universitas Islam Indonesia, Indonesia		

[Details of activities]

1. Research outline and its perspective

   I have been attended to the conference (PACCON2024 (The 2024 Pure and Applied Chemistry International Conference) and visited Assist. Prof. Ganjar Fadilah who are the member of IROAST research cluster in Indonesia. At the PACCON2024, I have introduced our recent research as Invited lecture then discussed with the professors. Prof. Wang from Xiamen University, China is very interested in my talk and future collaboration research about metals in cell analysis are discussed. Also, the committee member of the conference, Assoc. prof. Attitaya and I have discussed about the metal nano-particle analysis, especially elution from the products. And we have agreed to apply the grant for Bilateral Collaborations. After the conference, I have visited Assist. Prof. Ganjar. Also, Assist. Prof. Rahmat (who was visited Kumamoto Univ. as internship) joined to us with his family. We have discussed about the research on molecular imprinted material for ionic solute analysis and applying to MEXT scholarship for Mr. Rahmat.

(LEFT) With Prof. WANG, Prof. Attitaya and her students
(Right) With Associate Profs. Ganjar, and Rahmat and his familly

2. Research progress and results in the fiscal year
   For the metal nano-particle analysis, we have developed the new pretreatment method which can improve the detectable size of the particle. The progress was applied to the patent and presented at the conference. About the molecular imprinted membrane, the selectivity for amino acids, and ionic solutes were dramatically improved. Furthermore, the chiral separations for amino acids are achieved not only for phenylalanine but also for branched chain amino acids.

3. Research plan for the next year
   Metal nano-particle analysis will be further optimized for the effective separation of charged particulates. After the optimization, the manuscript will be prepared and submitted. Furthermore, the proposal for the grant aided for Bilateral Collaborations (JSPS) will be prepared.
   Amino acid analysis for blood test will be developed. The several targeted analyzer will be designed, established and evaluated. The evaluation will be performed with conventional analysis system, hplc. Furthermore, the chiral separation system will be established for the purification of pharmacy and/or their materials.

4. List of journal papers (with IROAST as your affiliation) published between April 2023 and March 2024.

   Ganjar Fadillah, Kei Toda, Shin-Ichi Ohira, One-stage chiral enrichment process by continuous flow electrodialysis with molecularly imprinted membrane, *Separation and Purification Technology*, **305**, 122492 (2023)

   Rahmat Hidayat, Ganjar Fadillah, Shin-Ichi Ohira, Glass tube-coated TiO_2 nanostructure for degradation of methylene blue: an experimental and design of column photocatalytic reactor, *Indonesian Journal of Chemical Analysis (IJCA)*, **6**(1), 52–62 (2023).

5. List of awards, grants, and patents
   [Patent]
   Analysis system and method for ionic solutes in ultra-pure water P7310867 (2023/7/10)

   [Grants]
   Adaptable and Seamless Technology transfer Program through Target-driven R&D (A-STEP) from Japan Science and Technology Agency (JST) Grant Number JPMJTR23RH.
   “Development of ultra-trace elemental analysis by means of ion-exchange with liquid electrode plasma”

Researcher Supported by the IROAST International Joint Research Travel Support Program

3-2-9	Adsorption studies of alkali and alkaline earth metal ions on zirconium metal–organic frameworks		
Name	Reetu Rani	Title	Postdoctoral Researcher
Affiliation	IROAST Email: ranireetu@kumamoto-u.ac.jp		
Period of Travel	February 18, 2024- February 25, 2024		
Visited Researcher	1) Thawatchai TUNTULANI 2) David J. HARDING	Title	1) Professor 2) Associate Professor
Affiliation	1) Chulalongkorn University, Thailand 2) Suranaree University of Technology, Thailand		

[Details of activities]

1. Research outline and its perspective
   Alkali and alkaline earth metal ions in different matrices pose significant environmental and health concerns. Therefore, there is a pressing need for materials exhibiting superior extraction/adsorption capabilities towards these ionic solutes. Metal organic Frameworks (MOFs), characterized by their porous structure, high surface area, tunable pore size and ease of functionalization, emerge as promising materials for such applications. In this study, the adsorptive behavior of alkali (Li, Na, K) and alkaline earth metal ions (Mg, Ca and Sr) was investigated with zirconium MOF; UiO-66-$COOH_2$ which has critical implication for design of membranes for separation of these metal ions.

2. Research progress and results in the fiscal year
   During this fiscal year, we successfully synthesized Zr-MOFs and tested the adsorptive behavior of carboxyl functionalized Zr-MOF towards alkali and alkaline earth metal ions and the results were presented at 9th Asian Conference on Coordination Chemistry (ACCC9) hosted in Bangkok, Thailand. In addition to presenting my work, I also engaged in discussions about the challenges and potential solutions in my research field.

3. Research plan for the next year
   The material (UiO-66-$COOH_2$) exhibits notable adsorption capabilities towards various metal ions present in aqueous solutions. Our next step involves evaluating its adsorption efficiency in real-world samples. Additionally, we intend to submit our preliminary research findings to esteemed international journals, necessitating the preparation of manuscripts for publication.

4. List of journal papers (with IROAST as your affiliation) published between April 2023 and March 2024.
   M. Garg, **R. Rani,** V.K. Meena, S. Singh, *Significance of 3D printing for a sustainable environment, Materials Today Sustainability*, 23, 1100419 (2023).

5. List of awards, grants, and patents
   Kumamoto University Financial Support for Female Researchers FY2023 for "Sample matrices isolation for ultra-trace metal analysis in sea water by means of metal organic frameworks-based membranes."

Researcher Supported by the IROAST International Joint Research Travel Support Program

3-2-10	Nanomaterials processing for medical, cosmetic, and environmental applications		
Name	Mitsuru SASAKI	Title	Associate Professor
Affiliation	Institute of Industrial Nanomaterials (IINa) Email: msasaki@kumamoto-u.ac.jp		
Period of Travel	September 9, 2023 - September 16, 2023		
Visited Researcher	1) PPC-2023, Barcelona (Spain), Sep. 11-12, 2023 2) ISHA2023, Valladolid (Spain), Sep. 12-14, 2024	Title	
Affiliation	1) Hall at the Hotel Sant Boi, Barcelona, Spain 2) University of Valladolid, Valladolid, Spain		

[Details of activities]

1. Research outline and its perspective.
   The aim of this travel to Spain was to attend the following two international conferences and delivered invited lectures on PPC conference, and keynote lectures on ISHA2023, respectively.
   (1) 3rd Global Conference on Polymers, Plastics, and Composites (PPC2023) at Sep. 11-12, 2023 in Barcelona, Spain.
   https://polymers-plastics.org/

   (2) International Solvothermal and Hydrothermal Association Conference (ISHA2023) at Sep. 11-14, 2023 in Valladolid, Spain.
   https://www.isha.website/

2. Research progress and results in the fiscal year
   In the PPC2023 conference, I delivered an invited talk entitled “Synthesis of silver nanoparticles/poly(N-isopropylacrylamide) composites for biomedical applications using pulsed arc discharge”, and got several questions. After the conference, I had chances to discuss with professors or presidents.
   From Sep 11 and Sep 13, I joined the ISHA2023 conference to deliver the Keynote talk entitled by “New Vinegar Production from Vinegar Processing Residue by the Subcritical Water Hydrolysis and Acetic Fermentation”. There were more than 10 questions to my talk right after my talk. I suppose that this kind of research topic is rare and very important for audiences.

3-2-11	Development of functional materials based on metal complex		
Name	Yoshihiro SEKINE	Title	Associate Professor
Affiliation	Priority Organization for Innovation and Excellence Email: sekine@kumamoto-u.ac.jp		
Period of Travel	July 22, 2023-July 27, 2023		
Visited Researcher	The 12th International Symposium on Nano & Supramolecular Chemistry (ISNSC-12)	Title	
Affiliation			

[Details of activities]

1. Research outline and its perspective

   Using this support program, I joined the international conference of "The 12th International Symposium on Nano & Supramolecular Chemistry (ISNSC-12)" as an invited speaker. It has several parallel scientific sections, and I have mainly attended the "Coordination Chemistry, and Supramolecular Chemistry" section to obtain information on scientific topics and trends, and do a discussion about my research topics of "Development of functional materials based on metal complex". During this conference, I discussed with Prof. Annie K. Powell from Karlsruhe Institute of Technology, and Prof. David J. Harding from Suranaree University of Technology the specific measurement methods and the details of synthetic strategy for functional coordination metal complexes.

2. Research progress and results in the fiscal year

The creation of molecular devices with high functionality, low environmental impact, low energy consumption, and simple manufacturing processes will have a great impact on a wide range of fields and industries and is one of the innovative technologies in the material properties required for the future society. Ferroelectric memory is another important target for next-generation molecular devices, and inorganic oxides such as perovskite-type oxides and ceramic ferroelectrics are the focus of research. Although various polar materials have been developed, the properties and degrees of freedom of electrons have not been fully utilized in the mechanism of polarization change of polar materials currently in use. In this study, we focus on the polarization function of polar materials, which is one of the most important functions of materials and widely used in society, and aim to create electron spin dynamics of stimulus-responsive coordination complexes. We will synthesize coordination complexes that can change their electronic and spin states and structures in response to external stimuli, achieve control of electric polarization by a new mechanism, and explore concerted magnetic and electric functions.

In my research, I have recently successfully synthesized the target complex. From the crystal structural analyses and temperature-dependent magnetic property measurements, that compound exhibited thermally induced electron transfers. Such a compound is a good candidate for polar materials.

3. Research plan for the next year

The final goal is to fabricate the functional materials exhibiting external-stimuli-responsive electrical dipole change. I will find the systematic synthetic methods for a series of functional materials, and investigate on their physical properties.

3-2-12	Study of Electrical Properties on interface of Silicon-Graphene Using First-Principles Molecular Dynamics Simulations and Implementation for Robust Machine-Learning Interatomic Potentials		
Name	Kohei SHIMAMURA	Title	Assistant professor
Affiliation	FAST Email: shimamura@kumamoto-u.ac.jp		
Period of Travel	Dec. 26, 2023 - Jan. 8, 2024		
Visited Researcher	Prof. Priya VASHISHTA	Title	Professor
Affiliation	University of Southern California		

[Details of activities]

1. Research outline

We conducted researches using first-principles molecular dynamics (FPMD) simulations and using machine-learning interatomic potentials (MLIPs). Charge transfer rate of Si-Graphene mixed system was investigated using non-adiabatic FPMD method. This study is important in order to clarify the factors of negative resistance known experimentally in the system. For MLIP, the development of graph neural network type (GNN-type) MLIP using the active learning and potential averaging methods and the implementation of thermal conductivity calculations were discussed. The former is necessary to realize robust MD simulations using the GNN-type MLIPs, and the latter plays an important role in calculating thermal conductivity with high accuracy for various materials.

2. Research progress and results in the fiscal year

[Non-adiabatic FPMD simulations of Si-Graphene system]

When voltage is applied from Si to Graphene in their bonded system, current flows from Si to Graphene. However, it has been experimentally shown that even if a low voltage is applied from Graphene to Si, current flows from Si to Graphene [i]. In order to clarify the factors behind this negative resistance, we performed non-adiabatic FPMD simulations [ii], and the charge transfer rates of hole and excited electron from Si to Graphene were estimated. It was found that the factor of negative resistance is that the charge transfer rate of the hole exceeds that of the electron.

[i] R. Ahsan, *et al.*, Europe PMC, rs-2935296/v1 (2023).
[ii] F. Shimojo, *et al.*, J. Chem. Phys., **140**, 18A529 (2014).

[Applications of GNN-type MLIPs]

We concentrate on the Allegro model [iii] that has been recently proposed. This MLIP employs a descriptor that is logically sound from a physical standpoint, featuring equivariance to the Euclidean group (consisting of translation, rotation, and mirror-image reversal symmetries). Even with limited training data, Allegro is able to show highly accurate results. We aimed to develop the introduction of active learning and potential averaging methods to construct a robust Allegro. We also attempted to implement a thermal conductivity calculation for allegro.

[iii] A. Musaelian, *et al.*, Nat. Commun., **14**, 579 (2023).

[For a robust Allegro model using active learning and potential averaging methods]

Both active Learning and potential averaging methods use multiple MLIPs with different

weights. The former calculates the standard deviation from the output of multiple MLIPs, and it is useful as an indicator for finding untrained structures through MD simulations. The latter is a method that performs MD simulation using the average value of the outputs of multiple MLIPs, improving the stability of the simulation. We demonstrated that a combination of these two methods constructed the highly robust MLIP based on feed forward NN (FFNN) [iv]. Allegro, which is based on GNN, can construct more sophisticated descriptors than that of FFNN, so we expect that the Allegro with two methods would show more accurate. However, since the number of weights of Allegro is quite large, unlike the FFNN-type MLIPs, applying the two methods to Allegro would result in extremely high computational costs. Incidentally, the number of weights in FFNN-type MLIP is ~10,000, while that in GNN type reaches as many as 1 million. We therefore proposed to introduce different weights for only one part of the Allegro, and to use weights commonly in multiple Allegros for most of the rest. Allegro uses most of weights for creating descriptors, and in the final process one FFNN is used to convert the descriptors to energy. We believe that trying to implement this FFNN with different weights is a good way to reduce the computational cost.

[iv] D. Wakabayashi, *et al.*, J. Phys. Soc. Jpn., **92**, 054005 (2023).

[Thermal conductivity calculation using Allegro]

Allegro has the advantages of having advanced descriptors and being very easy to adjust them compared to conventional MLIPs. These are useful for finding thermoelectric material candidates with low thermal conductivity. Since the thermoelectric materials show highly anharmonic dynamics, a sophisticated descriptor that can extract the characteristics of their behavior is required. We aimed to develop a thermal conductivity calculation method based on the Green-Kubo formula (GK method) using Allegro. This is because the GK method can calculate the thermal conductivity of any system. However, Allegro is not implemented to calculate the heat flux required for the GK method. Therefore, we extended allegro based on knowledge from our previous studies [v]. We adopted Ag_2Se as a test system to demonstrate the correctness of our implementation.

[v] K. Shimamura, *et al.*, Chem. Phys. Lett., **778**, 138748 (2021).

3. Research plan for the next year

[Non-adiabatic FPMD simulations of Si-Graphene system]

[Thermal conductivity calculation using Allegro]

We plan to publish the results in papers.

[For a robust Allegro model using active learning and potential averaging methods]

We will modify the FFNN part of Allegro to enable active learning and potential averaging methods, and then evaluate the computational cost.

4. List of journal papers

1. D. Wakabayashi, *et al.*, J. Phys. Soc. Jpn., **92**, 054005 (2023).
2. K. Shimamura, *et al.*, Comp. Phys. Commun., **294**, 19258 (2024).

5. List of grants

JSPS KAKENHI Grant Number 22K03454.