3-2. IROAST International Joint Research Travel Support Program

No.	Name	Destinations Period
3-2-1	**Muhammad Sohail AHMAD** IROAST	The University of Adelaide, Australia September 30, 2024 – October 12, 2024
3-2-2	**Shaojie GU** MRC	Zhejiang University, China January 12, 2025 – January 17, 2025
3-2-3	**Kei ISHIDA** CWMD	Middle East Technical University, Turkey August 27, 2024 – September 8, 2024
3-2-4	**Makiko KOBAYASHI** FAST	Anglia Ruskin University, UK March 4, 2025 – March 8, 2025
3-2-5	**Kwangsik KWAK** FAST	Karlsruhe Institute of Technology, Germany November 17, 2024 – November 24, 2024
3-2-6	**Ruda LEE** IINa	Sungkyunkwan University (SKKU), Korea August 6, 2024 – August 31, 2024
3-2-7	**Ruda LEE** IINa	1) Korea Advanced Institute of Science and Technology (KAIST), Korea 2) Chonnam National University, Korea 3) Korea Research Institute of Chemical Technology (KRICT), Korea October 27, 2024– November 7, 2024
3-2-8	**Mohammad Atiqur RAHMAN** IROAST	International Congress on Catalysis, France July 12, 2024 – July 23, 2024

3-2-9	**Atsushi SAINOKI** FAST	The University of Nouakchott, Mauritania October 6, 2024 – October 25, 2024
3-2-10	**Yoshihiro SEKINE** POIE	Kyungpook National University, Korea August 29, 2024 – September 5, 2024
3-2-11	**Kohei SHIMAMURA** FAST	University of Southern California, USA August 18, 2024 – August 31, 2024
3-2-12	**Kohei SHIMAMURA** FAST	University of Southern California, USA December 25, 2024 – January 8, 2025
3-2-13	**Masayuki TANABE** FAST	University of Southern Queensland, Australia December 10, 2024 – December 20, 2025

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

FAST：Faculty of Advanced Science and Technology

IINa：Institute of Industrial Nanomaterials

MRC：Magnesium Research Center

POIE：Priority Organization for Innovation and Excellence

No.3-2-1	Hydrogen production through photocatalytic biomass conversion		
Name	Muhammad Sohail AHMAD		
Affiliation	IROAST Email: Sohail@kumamoto-u.ac.jp	Title	Specially Appointed Assistant Professor
Period of Travel	September 30, 2024 - October 12, 2024		
Visited Researcher	Dusan LOSIC		
Affiliation	The University of Adelaide, Australia	Title	Professor

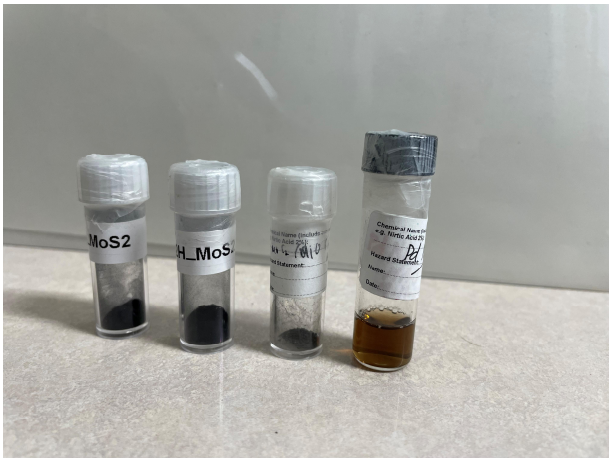
[Details of activities]

The primary purpose of my visit to the University of Adelaide specifically the Losic group and Cameron group was to explore collaborative research opportunities and interact with faculty and researchers in my field of study. This visit also provided me with insights into the research infrastructure and academic environment of the university. I presented a lecture titled "Functionalization of Graphene oxide for Catalysis and Energy Applications" focusing on how we can strengthen collaboration between our research groups. We had the opportunity to have prepare a material based on molybdenum disulfide and palladium doped molybdenum disulfide.

Engaging discussions and collaborative insights with the Losic group at the University of Adelaide

The palladium-doped molybdenum disulfide (PdMoS) is a highly promising material for catalysis, particularly in hydrogen evolution reactions (HER). MoS, while widely studied, suffers from low conductivity and inactive basal planes. Doping with palladium enhances its electrical conductivity and increases the number of active catalytic sites, improving hydrogen adsorption and dissociation. This modification boosts the overall efficiency and stability of MoS_2 in electrochemical applications. PdMoS is typically synthesized through hydrothermal or chemical vapor deposition methods and is also explored for applications in gas sensing, CO_2 reduction, and organic catalysis.

PdMoS can be synthesized using methods such as hydrothermal synthesis and chemical vapor deposition (CVD). In the hydrothermal method, molybdenum precursors are mixed with palladium salts in a solvent and heated under high pressure. In CVD, metal precursors are vaporized and deposited onto a heated substrate, allowing palladium to integrate into the MoS structure. These synthesis techniques enhance the material's electrical conductivity and catalytic activity, making PdMoS suitable for various applications, including hydrogen evolution reactions.



Synthesized samples based on MoS

I had productive discussions with Professor Dusan Losic and other faculty members regarding potential collaborative research on graphene-based membranes, catalytic chemistry. We exchanged ideas on future research directions and opportunities for joint publications or research projects.

The synthesized PdMoS will be characterize to evaluate its structural, electrical, and catalytic properties. Techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), and electrochemical testing will be employed to assess the material's performance and stability. The findings from this research will contribute to a collaborative paper highlighting the advancements in PdMoS for catalytic applications. We aim to submit the manuscript to a reputable journal, focusing on original contributions to the field of materials chemistry and catalysis.

Discussion with professor Losic

No.3-2-2	Exploring the Principles and Applications of Material Modification Using Electron Wind Force		
Name	Shaojie GU	Title	Assistant Professor
Affiliation	Magnesium Research Center Email: shaojie.gu@mech.kumamoto-u.ac.jp		
Period of Travel	January 12, 2025 - January 17, 2025		
Visited Researcher	Yang JU	Title	Professor
Affiliation	Zhejiang University, China		

1. Research outline and its perspective

The joint research aims to optimize microstructures and enhance the performance of advanced manufacturing materials through electron wind force while developing a control theory (**Fig. 1** Research exchanges). By exploring the impact of electron wind on defects (e.g., dislocations, grain boundaries, cracks) via in-situ experiments, the study seeks to clarify the thermal and athermal effects of current treatment, establishing a framework for industrial applications.

2. Research progress and results in the fiscal year

Through this international collaborative research, both parties shared their respective research progress. Together, we have gained a preliminary understanding of the optimal conditions for current healing techniques.

3. Research plan for the next year

In the coming fiscal year, we plan to conduct in-situ observation experiments to investigate the microstructural evolution under current treatment. Additionally, we will work collaboratively to develop a control theory linking current-induced microstructure optimization with performance enhancement.

4. List of journal papers

Regarding this collaboration, we are in the process of preparing research results and papers, where we will acknowledge the financial support provided by IROAST.

5. List of awards, grants, and patents

The partner team highly recognized my research progress and honored me with a certificate of recognition (**Fig. 2**). Additionally, we aim to explore the potential for further intellectual property development and grant applications based on this collaborative research.

Fig. 1 Research exchanges

Fig. 2 Awarded honorary certificates

No.3-2-3	Deep Learning for Hydrology		
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	August 27, 2024 - September 8, 2024		
Visited Researcher	Ali ERCAN	Title	Associate Professor
Affiliation	Middle East Technical University, Turkey		

[Details of activities]

1. Research outline and its perspective

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 late August to early September, I visited Middle East Technical University (METU) in Turkey to advance my collaborative research with Professor Erican (Figure 1). On the first day of my visit, we toured the terrain and rivers around Ankara, focusing on Lake Tuz (Figure 2), which has been experiencing a decline in water levels due to the effects of global warming. From the second day onward, we concentrated on writing a paper based on our collaborative research results. Since last year, we have been analyzing global atmospheric data for both past and future periods, which are used as inputs for deep learning models. We have calculated statistics and indices for various variables from this atmospheric data and analyzed them. We are now drafting a paper based on one of these results, specifically focusing on the aridity index calculated from the atmospheric data. During my stay, we discovered errors in one of the variables in the original atmospheric dataset. As a result, we recalculated the variable ourselves using other variables (Figure 3). Meanwhile, we divided the paper into sections and worked on writing each part separately. We hope to finalize it soon.

Figure 1. Faculty Dining Hall of METU

Figure 2. Salt lake near Ankara

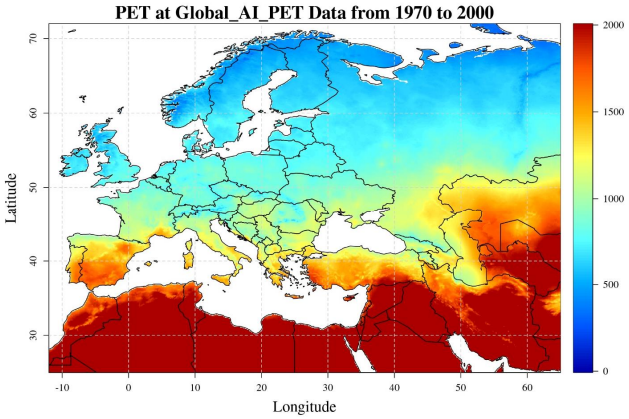


Figure 3. Evapotranspiration over Europe

No.3-2-4	Development of Wearable Ultrasound Sensors for Next-Generation Healthcare		
Name	Makiko KOBAYASHI	Title	Professor
Affiliation	Faculty of Advanced Science and Technology Email: kobayashi@cs.kumamoto-u.ac.jp		
Period of Travel	March 4, 2025 - March 8, 2025		
Visited Researcher	Oliver FAUST	Title	Associate Professor
Affiliation	Anglia Ruskin University, UK		

[Details of activities]

1. Research Outline and Perspective

This research aims to apply ultrasonic/piezoelectric sensing technology to the medical field by using wearable sensors for real-time physiological monitoring. We focus on device wearability, measurement accuracy, and the development of data analysis methods, with applications in telemedicine and home care in mind. Through this visit, we plan to strengthen collaboration among team members, establishing a sustainable, interdisciplinary research framework.

2. Research Progress and Results in the Current Fiscal Year

I and Prof. Oliver met several professors, such as Professor Marcian Cristea, Head of the School of Computer Science, Professor Laurie T Butler, Pro Vice Chancellor and Dean Faculty of Science & Engineering, Professor Yonghong Peng, Dean of Research Faculty of Science & Engineering, for MOU agreement and joint grant applications. We submitted joint UK grant, International Exchanges 2025 Global Round 1, in March 2025.

3. Research Plan for the Next Year

Aim to further enhance the performance of the wearable ultrasonic sensor and expand its potential applications by upgrading the device and testing prototypes and to integrate the advanced data analysis methods (AI, machine learning, etc.) to fully leverage measurement data and explore possibilities for telemedicine and home care, we will sign MOU and submit Aspire, Japan-UK joint call for collaborations in Advancing Human-Centered AI.

4. List of Journal Papers Published or Planned for Publication Between April 2024 and March 2025

Currently preparing a manuscript. We plan to present at conferences and submit for publication within 2025.

5. List of Awards, Grants, and Patents

None.

No.3-2-5	Tribological and mechanical properties of a laser powder bed fusion processed 316L		
Name	Kwangsik KWAK	Title	Assistant Professor
Affiliation	Faculty of advanced science and technology Email: kwak@msre.kumamoto-u.ac.jp		
Period of Travel	November 17, 2024 - November 24, 2024		
Visited Researcher	Martin DIENWIEBEL	Title	Professor
Affiliation	Microtribology center, Institute for applied materials IAM, Karlsruhe Institute of Technology, Germany		

[Details of activities]

1. Research outline and its perspective

Additively manufactured 316L stainless steel by laser powder bed fusion (LPBF-316L) has attracted much attention in various industrial fields, such as aerospace, automobile, marine, and medical industries, because of its excellent mechanical properties, biocompatibility, and corrosion resistance. Since the microstructure of the LPBF-316L varies according to the manufacturing parameters, such as laser power, scan speed, and the thickness of a layer, the mechanical properties depending on the microstructure are also variable. Increasing the laser power improves the resistance to friction and wear because of the increase in density and hardness of the material. However, it may result in anisotropy in the mechanical properties owing to a strong texture according to the columnar grains developed in one direction. Moreover, the austenite phase in stainless steel can be transformed into the martensite phase by the deformation-induced transformation. Therefore, it is essential to understand the influence of the transformed martensite phase on the friction and mechanical properties. This study aims to investigate the friction properties of the LPBF-316L and elucidate the effects of the transformed martensite on the friction properties. Friction properties will be measured using a micro-tribometer (Fig.1) at Karlsruhe Institute of Technology (KIT), Germany, and the bending properties will be measured using a micro-bending testing machine (Fig. 2) from Kumamoto University.

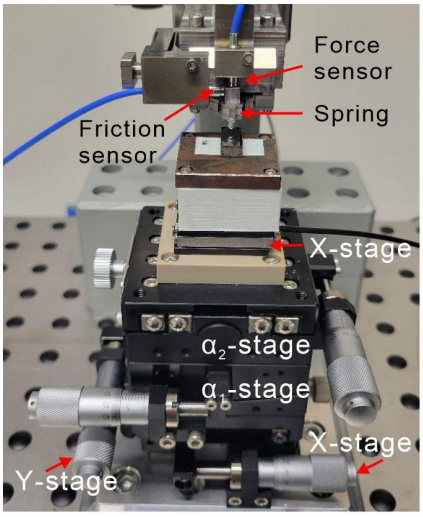


Fig. 1 Micro-tribometre

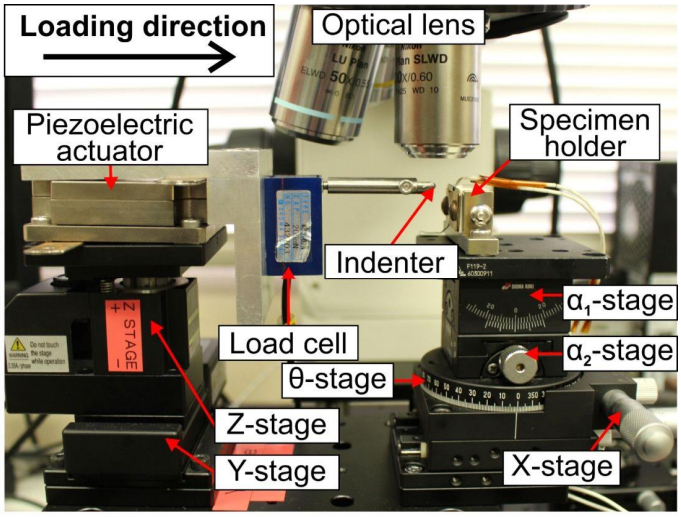


Fig. 2 Micro-bending testing machine

2. Research progress and results in the fiscal year

The material used in this study was stainless steel 316L produced by laser powder fusion bed. The friction tests were performed using a micro-tribometre at Karlsruhe Institute of Technology (KIT) in Germany. 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 = 1.938 and kN = 5.062 mN / μm. The micro-friction tests were performed in dry contact at room temperature, an air atmosphere, and normal ambient humidity. The normal forces of 60, 80, 90, and 100 mN were loaded in a Z direction on the X plane of the sample, which corresponded to 400, 450, 470, and 500 MPa of Hertzian contact pressure, respectively. For the 100 mN, the friction test that the normal force was loaded in the Y direction was also conducted. 1000 linear reversible cycles were conducted at a stroke length of 3 mm and speeds of 1.0 mm s-1. The normal and friction forces were measured continuously during the tests.

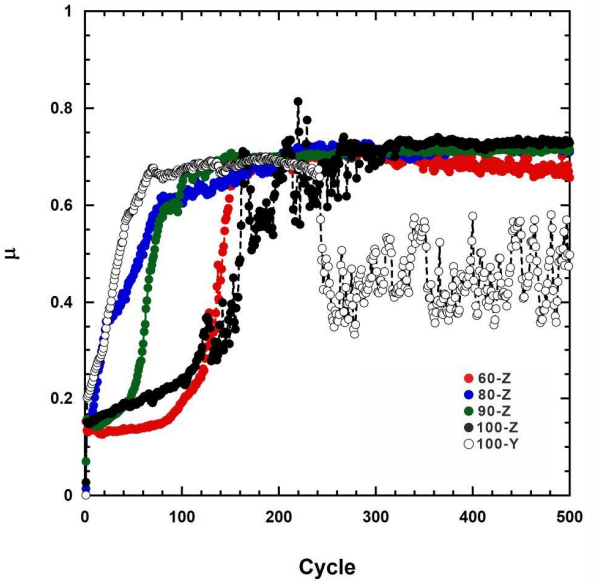


Fig. 3 Friction coefficient versus cycle. The number and alphabet in the index indicate the normal force and contact direction, respectively.

Fig. 3 shows the relationship between the mean coefficient of friction (CoF) and cycle. The CoF of the 60-Z, 80-Z, 90-Z, and 100-Z samples was almost constant, approximately 0.7, in a region of steady state, although the CoFs in the running-in period varied. This may be due to roughness or undulation of the sample surface. Meanwhile, in the normal force of 100 mN, the CoF of the Y-direction sample fluctuated between 0.35 and 0.6, similar to the 0.35±0.05 of 100Cr6 bearing steel. The CoF in soft materials is generally higher than that in strong materials. From this point of view, the strong fluctuation and low CoF values of the 100-Y samples may be attributed to the deformation-induced martensitic transformation. Although a similar phenomenon was also observed in the early stage of the friction behaviour of the Z-direction samples, the CoF in a steady state maintains a high value.

Fig. 4 shows the confocal images of the wear tracks after friction tests. As depicted in Fig. 3a, the black spots and friction traces on the wear track of the 100-Z were observed, which were also visible in 60-Z, 80-Z, and 90-Z samples. In contrast, in the 100-Y sample, the distinct friction traces were observed without the black spots. The width of the friction traces on the 100-Y was wider than that on the 100-Z. This finding indicates that the

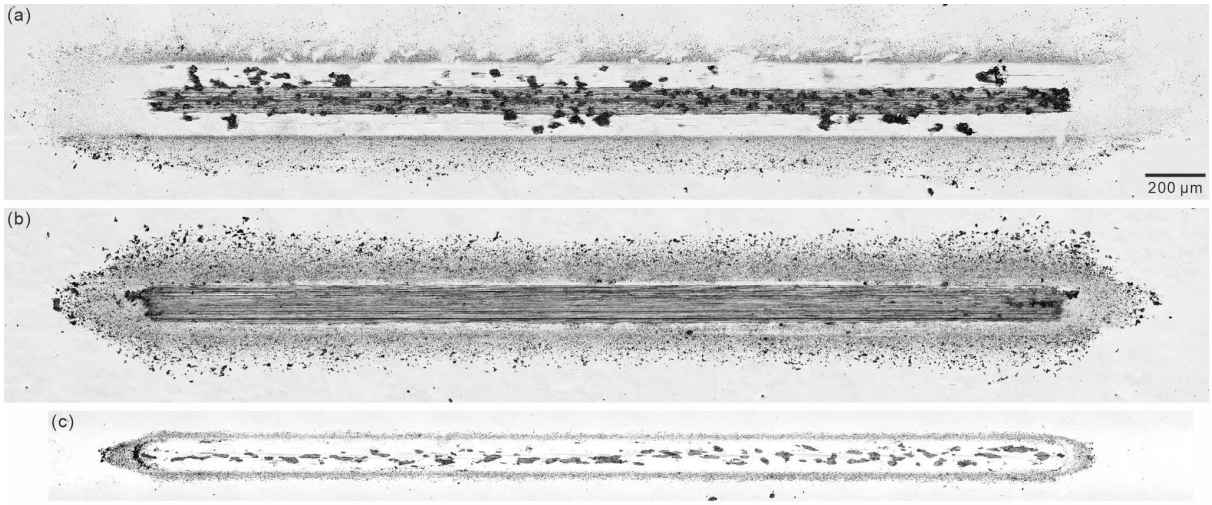


Fig. 4 Confocal images of the wear tracks after friction experiments with differing normal force or sliding direction: (a) 100 mN–Z, (b) 100mN–Y, and (c) 90 mN–Z.

deformation-induced transformation partially occurred in the early stages of the friction behaviour for loads of 100 mN or less and the Z-direction sliding, while in the Y-direction sliding, the deformation-induced martensitic transformation continuously occurred. This is probably due to the peculiar microstructure morphological features produced during the additive manufacturing process, such as columnar grains developed in one direction. We will clarify the effect of deformation-induced martensite microstructure on friction behaviour concerning the results of metallographic analysis.

3. Research plan for the next year

We will examine the microstructure observation of the wear tracks using an electron backscatter diffraction or transmission electron microscope. We will perform the micro-bending test using a cantilever specimen, which will be prepared from the transformed martensite phase using the focused ion beam machining. In FY2024, although the friction tests are performed in the air only. However, in FY2025, the friction tests will be conducted in a lubricating environment, and the influence of the martensite transformation on the bending properties will be investigated.

4. List of journal papers published between April 2024 and March 2025.

Not Applicable

5. List of awards, grants, and patents

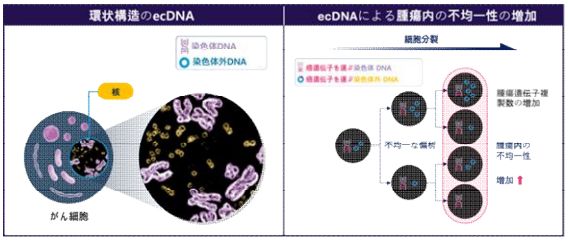
Not Applicable

No.3-2-6	Analyze the correlation between therapeutic effects of multidrug-resistant cancer and extrachromosomal DNA and predict disease prognosis		
Name	Ruda LEE	Title	Associate Professor
Affiliation	Institute of Industrial Nanomaterials Email: aeju-lee@kumamoto-u.ac.jp		
Period of Travel	August 6, 2024 - August 31, 2024		
Visited Researcher	Hoon KIM	Title	Associate Professor
Affiliation	Sungkyunkwan University (SKKU), Korea		

[Details of activities]

1. Research outline and its perspective

Discussions with experts from various fields have highlighted the relationship between multidrug resistance and chromosomes, revealing that correlation analysis involving extrachromosomal circular DNA (ecDNA) shows potential. However, as ecDNA research is still in its early stages and the academic framework is not fully developed, treating this topic as a standalone field poses challenges. Thus, interdisciplinary research that embraces multidisciplinary connectivity is essential. The research team aims to enhance foundational research capabilities for cancer prognosis and treatment prediction related to ecDNA and multidrug-resistant cancer cells through interdisciplinary collaboration, establishing an effective cooperation system. The primary goal of this research initiative is to secure foundational technology and develop treatment strategies by prioritizing innovative ecDNA technologies and achieving successful research outcomes through close collaboration.

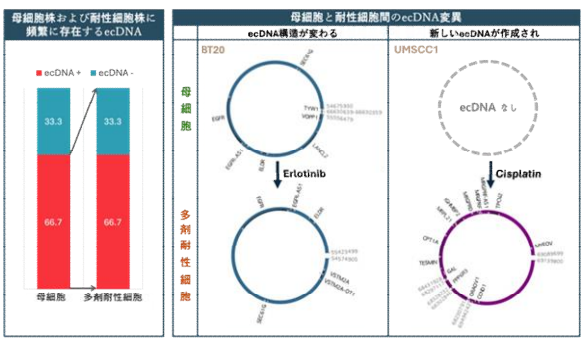


2. Research progress and results in the fiscal year

Based on the analysis results from the whole genome sequencing (WGS) data of the parental cell lines and chemoresistant tumor cell lines held by Lee LAb on the opposing side, it was confirmed that approximately 67% of the parental cell lines possess ecDNA, which aligns with the existing fact that ecDNA is frequently present in cancer cells. Additionally, among the resistant cell lines, 67% of the cells that possess ecDNA maintain it, suggesting a correlation between ecDNA and drug resistance.

3. Research plan for the next year

In our future plans, we aim to explore the potential for new drug development and industrialization. We intend to focus on developing new anti-cancer drug targets and treatment strategies to effectively tackle drug resistance. Leveraging our research findings, we plan to establish a foundation for the development of innovative technologies that can overcome drug resistance, ultimately



contributing to advancements in the domestic and international pharmaceutical industry.

4. List of journal papers published between April 2024 and March 2025.

Ruda LEE

1) Min Woo Kim, Sol Moon, Yong Il Park, Jungho Kim, Seung Il Kim, and **Ruda Lee***. Ultrasound-Responsive Lipid Nanoparticles for Targeted Therapy and Controlled Drug Release in Non-Small Cell Lung Cancer. *Adv. Therap.* 2024, 2400248. DOI: 10.1002/adtp.202400248
2) Jeon Geun Kim, Hyeon Jung Yu, **Ruda Lee***, and Yong Il Park*. Recent Developments in Near-Infrared-II Luminescence Imaging Using Inorganic Nanoparticles: Semiconductor Quantum Dots and Lanthanide Nanoparticles. *Korean J. Chem. Eng.* 2024; 41, 3603-3619. DOI: 10.1007/s11814-024-00300-4

Hoon KIM

1) Bum Soo Lee†, **Hoon Kim**†, Jiwon Baek, Rhim Ryoo, Seoung Rak Lee, and Ki Hyun Kim*. Determination of the Absolute Configuration of Secondary Alcohols in a Compound Mixture via the Application of Competing Enantioselective Acylation Coupled with LC/MS Analysis. *Pharmaceutics* 2024, 16(3), 364; DOI:10.3390/pharmaceutics16030364.
2) Dahyun Park, Sungho Bea, Ji-Hwan Bae, Hyesung Lee, Young June Choe, Ju-Young Shin, **Hoon Kim***. PCSK9 Inhibitors and Infection-Related Adverse Events: A Pharmacovigilance Study Using the World Health Organization VigiBase. *Drugs-Real World Outcomes* 11, 465–475 (2024). DOI: 10.1007/s40801-024-00430-5.
3) **Hoon Kim***, Soyeon Kim, Taylor Wade, Eunchae Yeo, Anuja Lipsa, Anna Golebiewska, Kevin C. Johnson, Sepil An, Junyong Ko, Yoonjoo Nam, Hwa Yeon Lee, Seunghyun Kang, Heesuk Chung, Simone P. Niclou, Hyo-Eun Moon, Sun Ha Paek, Vineet Bafna, Jens Luebeck & Roel G. W. Verhaak*. Mapping extrachromosomal DNA amplifications during cancer progression. *Nat Genet* **56**, 2447–2454 (2024). DOI: 10.1038/s41588-024-01949-7

5. List of awards, grants, and patents

Ruda LEE

1) FY2022 JSPS, Grant-in-Aid for Scientific Research (C)
2) Brain Pool Korea 2022

Hoon KIM

1) STEAM research; Pioneer, FY2022-FY2026
2) Basic Science Research (MRC), FY2019-FY2026
3) Center Research Hospital R&D, FY2024-FY2025
4) Senior Researcher Grant, FY2023-2028
5) Boston-Korea, FY2024-FY2029

No.3-2-7	Development of Novel Therapeutic Strategy Using Upconversion Nanoparticles for Head and Neck Cancer		
Name	Ruda LEE	Title	Associate Professor
Affiliation	Institute of Industrial Nanomaterials Email: aeju-lee@kumamoto-u.ac.jp		
Period of Travel	October 27, 2024-November 7, 2024		
Visited Researcher	1) Changhwan LEE 2) Yong Il PARK 3) Sang Hwan NAM	Title	1) Assistant Professor 2) Professor 3) Principal Investigator
Affiliation	1) Korea Advanced Institute of Science and Technology (KAIST), Korea 2) Chonnam National University, Korea 3) Korea Research Institute of Chemical Technology (KRICT), Korea		

[Details of activities]

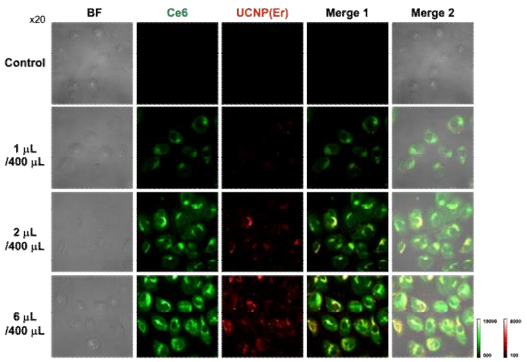
1. Research outline and its perspective

Cancer is a significant global health challenge, particularly because of the persistent issue of drug-resistant cancer cells that undermine conventional treatment efficacy. Upconversion nanoparticles (UCNPs) have emerged as promising candidates for cancer therapy due to their unique ability to convert tissue-penetrating near-infrared (NIR) light into higher-energy UV-vis) luminescence. This allows for the targeted treatment of solid tumors located in deep tissues, using minimally invasive techniques.

UCNPs offer distinctive advantages for multimodal imaging-guided cancer therapy, providing both therapeutic and diagnostic capabilities. Their unique optical properties make them an exciting new class of agents for tackling solid tumors and enhancing imaging contrast, leading to more precise tumor localization and monitoring. We propose to explore the photodynamic therapy (PDT) effects of UCNPs in treating drug-resistant cancer cells. Our goal is to investigate and understand how UCNPs can be utilized to overcome the defenses of drug-resistant tumors, thereby improving treatment outcomes and providing a new avenue for cancer therapy.

2. Research progress and results in the fiscal year

The material synthesis was initially conducted at Kumamoto University. Utilizing the NP synthesis protocol, the setup was successfully established at KRICT for the fresh preparation of the NPs. KRICT further purified the samples using a specially developed column and took TEM/PL images, confirming the co-localization of the UCNPs within the polymeric NPs. The KRICT lab installed multi-photon imaging devices, which were employed to set the conditions for NP internalization. The study varied key parameters, such as time points and concentrations, to identify the most effective conditions for PLGA/UCNPs-loaded NPs. With these conditions established, real-time tracking of NP internalization was performed using KRICT's imaging technology.



3. Research plan for the next year

Next year, we plan to optimize and scale up NP synthesis, conduct advanced imaging studies using multi-photon devices, initiate in vivo trials with MDR cancer models, strengthen collaborations for incorporating innovative techniques, and disseminate our findings through high-impact publications and conferences, all aimed at advancing effective treatments for multi-drug-resistant cancers.

4. List of journal papers published between April 2024 and March 2025.

Ruda LEE

1) Min Woo Kim, Sol Moon, Yong Il Park, Jungho Kim, Seung Il Kim, and **Ruda Lee***. Ultrasound-Responsive Lipid Nanoparticles for Targeted Therapy and Controlled Drug Release in Non-Small Cell Lung Cancer. *Adv. Therap.* 2024, 2400248. DOI: 10.1002/adtp.202400248
2) Jeon Geun Kim, Hyeon Jung Yu, **Ruda Lee***, and Yong Il Park*. Recent Developments in Near-Infrared-II Luminescence Imaging Using Inorganic Nanoparticles: Semiconductor Quantum Dots and Lanthanide Nanoparticles. *Korean J. Chem. Eng.* 2024; 41, 3603-3619. DOI: 10.1007/s11814-024-00300-4

Yong Il PARK

1) Min Woo Kim, Sol Moon, Yong Il Park, Jungho Kim, Seung Il Kim, and **Ruda Lee***. Ultrasound-Responsive Lipid Nanoparticles for Targeted Therapy and Controlled Drug Release in Non-Small Cell Lung Cancer. *Adv. Therap.* 2024, 2400248. DOI: 10.1002/adtp.202400248

Changhwan Lee

N/A

Sang Hwan Nam

N/A

5. List of awards, grants, and patents

Ruda LEE

1) FY2022 JSPS, Grant-in-Aid for Scientific Research (C)
2) Brain Pool Korea 2022

Yong Il Park

N/A

Changhwan Lee

N/A

Sang Hwan Nam

N/A

No.3-2-8	Engineering Zeolitic Imidazolate Framework Derived Mo-Doped Cobalt Phosphide for Efficient OER Catalysts		
Name	Mohammad Atiqur RAHMAN	Title	Postdoctoral Researcher
Affiliation	IROAST Email: atiqur@kumamoto-u.ac.jp		
Period of Travel	July 12, 2024 - July 23, 2024		
Visited Researcher	Bert CHANDLER, Pennsylvania University, USA	Title	Professor
Venue	International Congress on Catalysis, France		

[Details of activities]

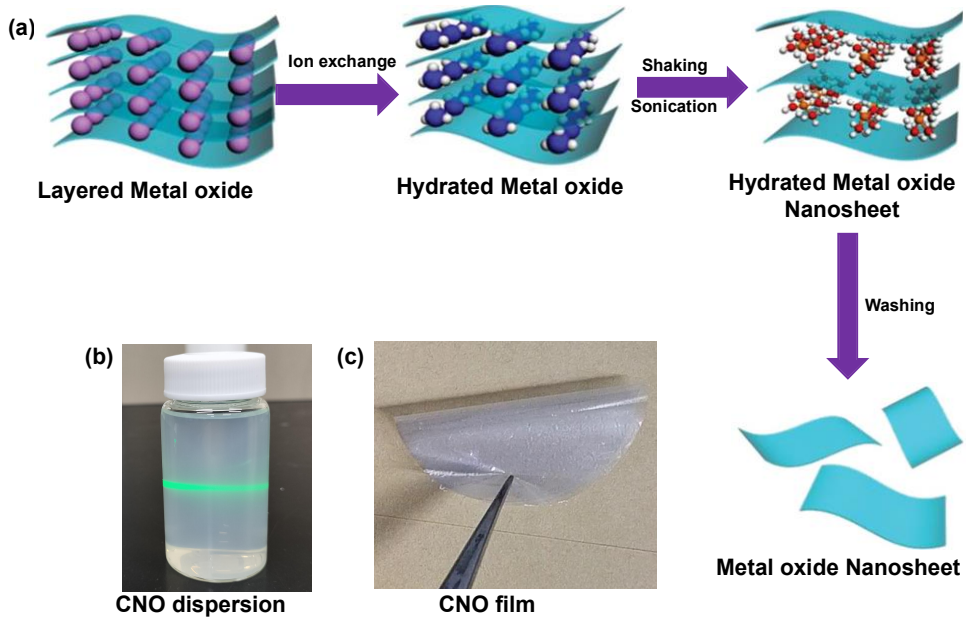
1. **Research outline and its perspective:**

I, Rahman Mohammad Atiqur, participated and presented my research work in the 18th International Congress on Catalysis (18th ICC) held at the Lyon Convention Centre, Lyon, France in July 2024. In this conference, I have presented my poster titled, "Engineering Zeolitic Imidazolate Framework Derived Mo-Doped Cobalt Phosphide for Efficient OER Catalysts". The poster session was started from 05:30 pm and ended at 07:30 pm. During this 2h period, I had opportunity to discuss about my research work with world reputed researcher from various universities. This discussion helps me to improvise my research capability and establish collaboration with the researcher from various institutions. In addition to presenting my research work I have also attended the plenary lecture on various themes including metal oxide-based catalysts, metal organic framework-based catalysts, organic-inorganic hybrid perovskite as visible light photocatalysts etc. and also involved with important discussion with the professor from various universities such as, Pennsylvania State University, United States, University of Liverpool, United Kingdom - Chinese Academy of Sciences, China etc. Moreover, I have also joined actively in the poster session which helped me to get new innovative idea and build up relationship with the researcher from my field. Furthermore, I have also engaged in establishing network with fellow researcher in related fields while exploring potential collaboration and future research opportunities.

2. **Research progress and results in the fiscal year**

(a) Synthesis of Calcium Niobium Oxide Membrane

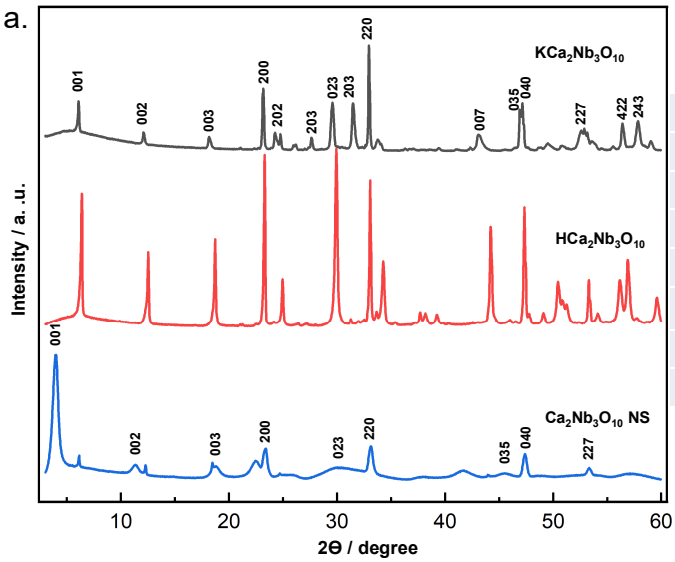
I have synthesized calcium niobium oxide (CNO) nanosheet by solid state reaction using K_2CO_3, $CaCO_3$ and Nb_2O_5 (ratio= 1.3:2:3) followed by proton exchange and delamination using tetrabutyl ammonium hydroxide (TBAOH). Membrane of these films was fabricated by vacuum filtration and ion exchange using hydrochloric acid (Scheme 1). The prepared CNO membrane has good flexibility and mechanical strength to be used as proton exchange membrane in proton exchange membrane fuel cell. The synthesized membrane was characterized using PXRD, XRF, AFM, and SEM to under its structural and morphological characteristics. Analysis of the results (Figure 2) suggests that the formation of CNO was successful. Additionally, observation of the cross-section SEM image indicates the layered structure of the CNO film obtained via vacuum filtration.



Scheme 1**:** (a) Synthesis strategy of metal oxide nanosheet; (b) CNO dispersion; and (c) CNO film fabricated by vacuum filtration.

Characterization:

The prepared materials have been characterized by XRD and XRF. From the PXRD pattern of the prepared material with the standard, it is clear that the resultant material was $K_2Ca_2Nb_3O_{10}$. Figure 2(a), (b), (c) and (d) shows the XPS spectra, morphology, thickness and layered structure of the prepared CNO nanosheet.



b. **XRF data**

	Mass%	mol%	
K	9.981	0.255279641	
Ca	22.341	0.557437996	
Nb	67.678	0.72845374	
	Relative %	**Formula Wt %**	**Formula**
	0.3504404	1.051321287	$KCa_2Nb_3O_{10}$
	0.7652346	2.295703756	
	1	3	

Figure 1: (a) PXRD pattern $KCa_2Nb_3O_{10}$, $HCa_2Nb_3O_{10}$ and $Ca_2Nb_3O_{10}$; (b) XRF data of $KCa_2Nb_3O_{10}$.

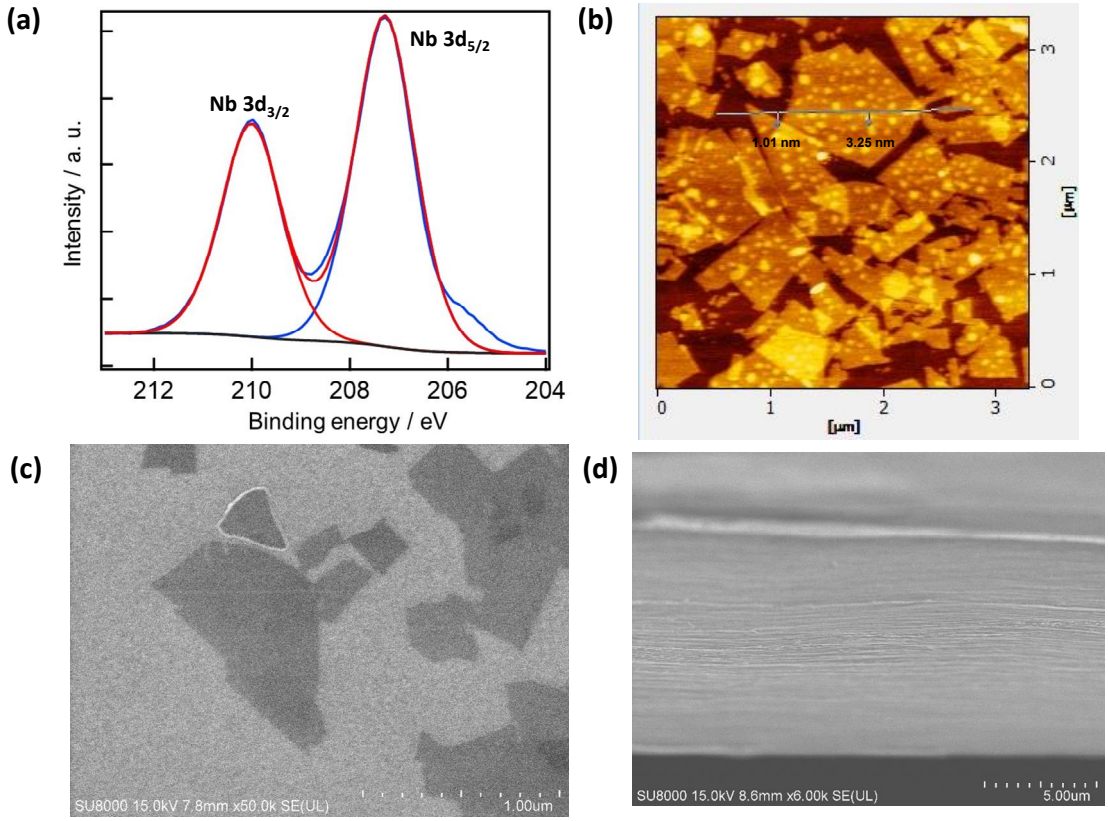


Figure2: (a) XPS 2d spectra of CNO; (b) AFM image of CNO; SEM image of CNO: (c) surface SEM, (d) cross section SEM.

Measurement of Proton Conductivity:

Proton conduction ability of the synthesized membrane as proton conductor was evaluated while tuning both humidity and temperature. I have found that CNO give rise to a proton conductivity of 4 $\times 10^{-6}$ S cm^{-1} at 50 ℃ and 60 % RH condition (Figure 3 (a). Under optimized condition, this membrane give rise to a proton conductivity of 4.21 $\times 10^{-5}$ S cm^{-1}. On the other hand, proton conductivity of CNO increases with the amount of Mg-dopant. Under optimized condition, MgCNO-3 give rise to a proton conductivity of 6.4 $\times 10^{-4}$ S cm^{-1}. Additionally, study of temperature dependence proton conductivity study showed the usual trend of the increase of proton conductivity with temperature. Calculation of activation energy showed that the proton conduction in CNO proceed via Grotthus mechanism. Finally, these membranes were utilized in proton exchange membrane fuel cell using CNO having various thickness and the results obtained shown in Figure 3 (d). When incorporated the CNO membrane having a thickness of 52 µm in proton exchange membrane fuel cell give rise to an optimum power density of 0.76 mW cm^{-2} while MgCNO-3 give rise to an optimum power density of 2.57 mW cm^{-2}. These results suggest that Mg-doping has an obvious effect on the proton conductivity and fuel cell performance.

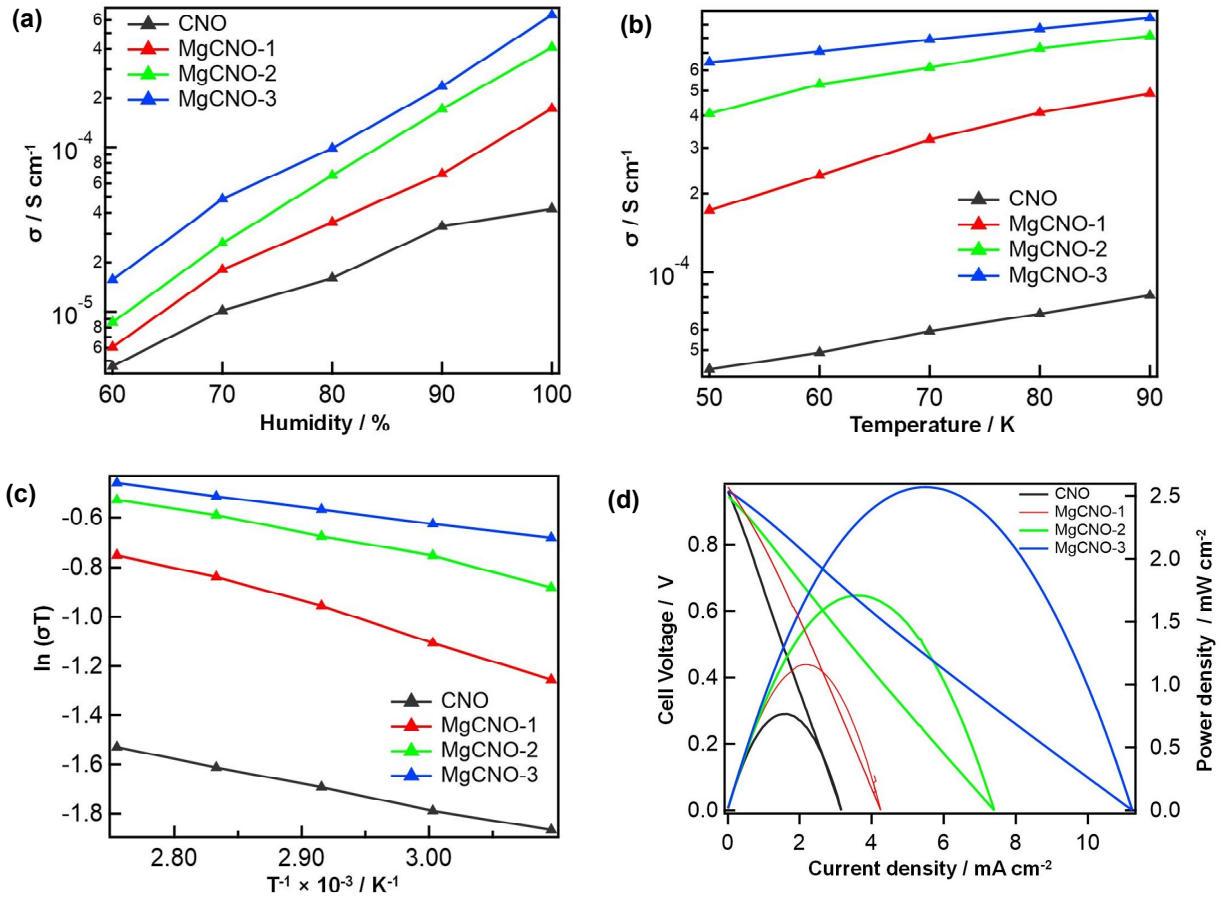
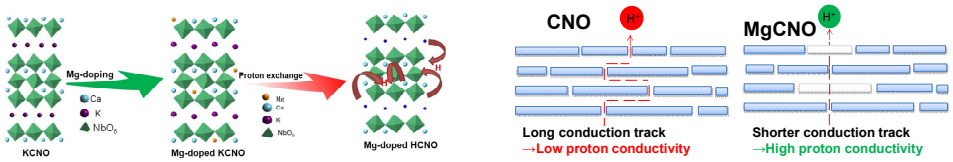


Figure3: Proton conductivity data of CNO and Mg-doped CNO in the out-of-plane direction: (a) Humidity dependent proton conductivity measured at 50 ℃; (b) Temperature dependent proton conductivity measured at 100 % RH condition, (c) Arrhenius plot; (d) Proton exchange membrane fuel cell performance of CNO and Mg-CNO measured at 80 degree and 100 % RH condition.

Mechanism of Proton Conductivity:

According to the activation energy calculation, proton conduction in CNO occurs via Grotthus mechanism. The effect of Mg-doping can be explained as follows:



Scheme2: Mechanism of proton conductivity in un-doped and doped CNO

3. Research plan for the next year

The demand for clean and sustainable energy resources has been soaring over the last few decades with the worldwide energy demand. Both these issues are obviously burning problems in terms of environmental pollution and increases in the average temperature of this planet. For this reason, development of clean and maintainable energy systems and advanced energy storage devices have become more significant than ever. In response to this, fuel cell, where electric energy is produced from chemical energy through an electrochemical reaction find interests by the researcher to fulfill the growing energy demands of newly emerging applications. Commercially Nafion has been used as electrolyte in fuel cell. Although they provide high proton conductivity, but strong humidity dependency and high price restrict their wide commercialization. Two-dimensional (2D) materials such as graphene, MoS2, montmorillonite, MXene, etc., have drawn attention from researchers all over the world in recent years due to their intriguing physicochemical properties. Among these 2D materials,

layered double hydroxide (LDH) nanosheets have found broad applications in electrochemical energy conversion devices due to their extraordinary performance and low price. LDH nanosheets can be exfoliated from the bulk phase of LDH, which is a type of anionic clay mineral material. LDH consists of positively charged host layers and interlayer equilibrium anions. The host layers of LDH possess a structure similar to hydro magnesite, consisting of a divalent cation octahedral structure surrounded by six hydroxyl groups, which form a continuous lamellar structure. The host layers of LDH undergo isomorphic substitution with trivalent cations, resulting in a positively charged host layer, while compensatory anions occupy the interlayer to maintain overall electroneutrality. LDH consists of both divalent and trivalent cations and these cations determine the surface charge of the host layer, while interlayer equilibrium anion and the water molecules associated with the LDH structure. The existence of these equilibrium anions endows LDH with anionic conductivity. This tunable ionic composition allows the utilization of different components LDH in various applications. In their natural state, LDH flakes tend to form agglomerates with a stacked lamellar structure due to electrostatic interactions between the host layers and the interlayer anions, as well as van der Waals forces and hydrogen bonding among the host layers. However, when exfoliated into single- or few-layer nanosheets, the properties of LDH nanosheets dramatically differ from their macroscopic state. Thus, fabrication of LDH nanosheet based electrolyte for application in fuel cell becomes Although researcher Therefore, researcher focused on the fabrication of LDH nanosheets based electrolyte for application in fuel cell. Although few researchers have reported about the fabrication of polymer and LDH nanosheet hybrid as proton and hydroxide ion exchange membrane for application in fuel cell. But fabrication of flexible LDH nanosheet membrane for application as electrolyte in proton exchange membrane fuel cell is not reported yet. Therefore, we are focusing on the fabrication of flexible LDH nanosheet membrane for application in proton exchange membrane fuel cell.

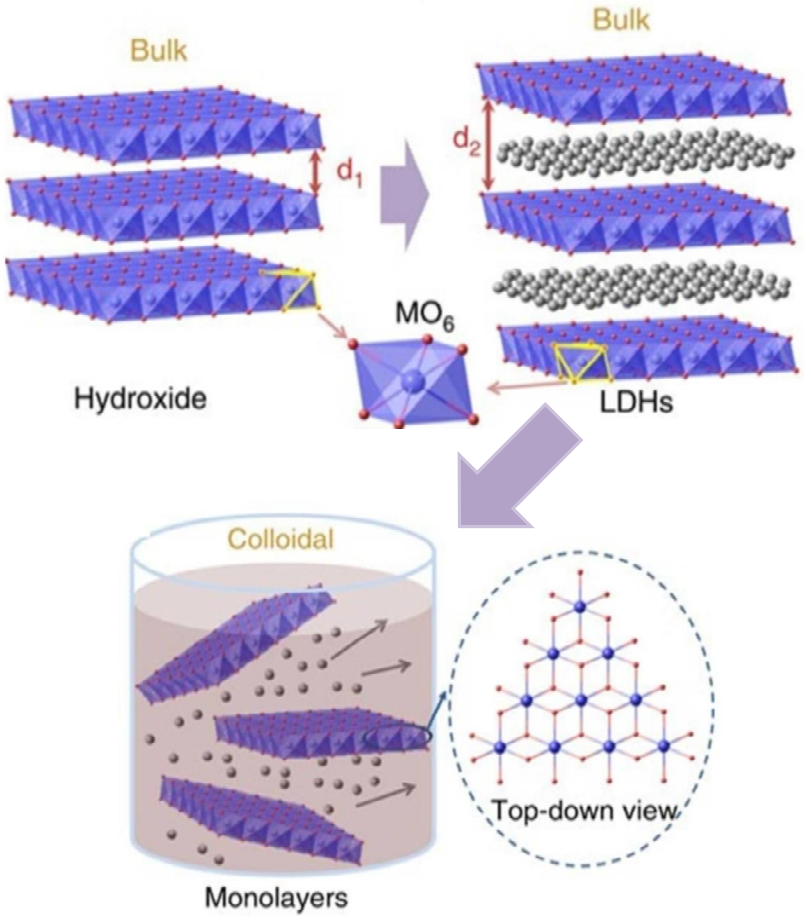


Figure 1: Schematic diagram of liquid-phase exfoliation of a typical layered double hydroxide

I am focusing on the following points:

- ❖ Synthesis and characterization of layered double hydroxide nanosheet.
- ❖ Effect various fabrication method on the characteristics of layered double hydroxide nanosheets.
- ❖ Different properties of the prepared nanosheets will be investigated to measure inherent properties for energy devices.
- ❖ Finally, this project will lead towards the achievement of carbon neutral society for achieving the SDGs.

4. List of journal papers published between April 2024 and March 2025.

[1]. Engineering Zeolitic-Imidazolate-Framework-Derived Mo-Doped Cobalt Phosphide for Efficient OER Catalysts, **Mohammad Atiqur Rahman**, Ze Cai, Zannatul Mumtarin Moushumy, Ryuta Tagawa, Yoshiharu Hidaka, Chiyu Nakano, Md. Saidul Islam, Yoshihiro Sekine, Yuta Nishina, Shintaro Ida, and Shinya Hayami*, *ACS Omega*, August 2024 (In Press).

[2]. Enhanced OH^- conductivity from 3D alkaline graphene oxide electrolytes for anion exchange membrane fuel cells, Nonoka Goto, **Mohammad Atiqur Rahman**, Md. Saidul Islam, Ryuta Tagawa, Chiyu Nakano, Muhammad Sohail Ahmed, Yoshihiro Sekine, Yuta Nishina, Shintaro Ida, and Shinya Hayami*, *Energy Advances*, 3(5), 1047-1053, 2024.

[3]. Ce-doped TiO_2 fabricated glassy carbon electrode for efficient hydrogen evolution reaction in acidic medium, Md. Nurnobi Islam, Md Mosaraf Hossain, Shrikant S. Maktedar,*Mostafizur, Rahaman, **Mohammad Atiqur Rahman**, Mohammad A. Hasnat*, *Chemistry—An Asian Journal*, e202301143.

Fig.1 : ICC-Lyon2024

Fig.2: Discussing about my research work during the poster session at the 18th ICC 2024

Fig.3: During the poster session at the 18th ICC 2024

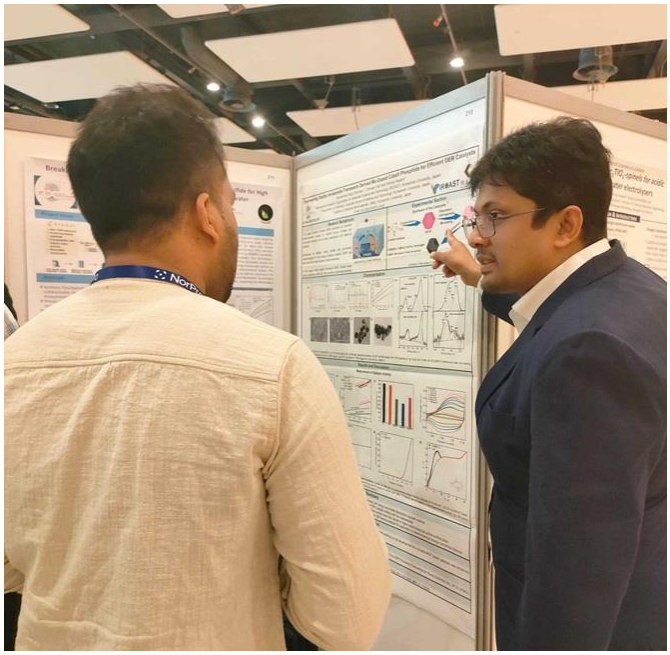


Fig.4: Discussing about my research work during the poster session at the 18th ICC 2024

No.3-2-9	Investigation of ASGM-induced mercury contamination in Chami and its environs, Mauritania		
Name	Atsushi SAINOKI	Title	Associate Professor
Affiliation	Faculty of Advanced Science and Technology Email: atsushi_sainoki@kumamoto-u.acjp		
Period of Travel	October 06, 2024 - October 25, 2024		
Visited Researcher	Ahmedou MAHFOUDH	Title	Professor
Affiliation	The University of Nouakchott, Mauritania		

[Details of activities]

Background

Gold from small-scale gold mines has been smelted in Chami, Mauritania, since 2016, but the problem here is the smelting method. As small-scale gold mines are developed by individuals rather than companies, there is little awareness of the environment, and the amalgamation method using mercury, which is cheap and simple, has been used in smelting. As a result, large amounts of mercury are discharged into the environment. In fact, this is a problem not only in Mauritania, but throughout Sub-Saharan Africa, where countless small-scale gold mines have been developed. A recent study reported that 80% of the 838 tonnes of mercury released into the environment annually is attributable to small-scale gold mines in Sub-Saharan Africa. Importantly, small-scale gold mines are present not only in Africa, but are being operated in more than 80 countries, estimated to support 15 million miners and the livelihoods of more than 100 million people. The problem is therefore of global scale and requires urgent action.

Sampling of soils

First, I stayed for a few days in the capital, Nouakchott to make a discussion on the sampling method and locations, obtain a permission letter from Prof. Ahmedou MAHFOUDH, The University of Nouakchott, and to prepare soil sampling apparatus in Chami. Then, I travelled 200 km north of Nouakchott to reach Chami on Thursday 10 October. There were no mountains or towns along the way, just endless horizontal terrain with gravel and sand deposits. I have been in many countries in the world, but this may be the first time I have seen the horizon.

On Friday 11 October, I first met with the district head (I am not sure if this is the correct term) who governs Chami. The district director has a strong interest in mercury pollution and promised full cooperation with the soil sampling. Then, I made preliminary visits to the area where I conduct soil sampling, to ensure that the soil sampling is conducted smoothly and examined the hardness of the soil to estimate the time required for sampling at one site.

From Saturday 12, October, to Tuesday 15, soil sampling was carried out as shown in Figure 1. This was extremely difficult work. First, a 40-cm-deep hole was dug at the sampling point, and soil samples were taken every 10 cm, after which pH and EC were measured. In addition, near-surface soil samples were taken at four points at north, east, south, and west locations located 5 m away from the centre hole and were weighed to 50 g for each. These operations had to be carried out in the middle of a desert/wilderness area

Figure 1: Soil sampling

where the temperature was close to 40°C. In addition, there was always a strong wind blowing from the north-east, so the whole body was covered. Although this sampling was significantly tiring and challenging, I was able to carry out soil sampling at about 50 sites. Importantly, this time, sampling was also carried out inside the gold smelter, which could not be done in the previous survey.

Preparation of sample exportation to Japan and discussion of research collaboration

I returned to Nouakchott, the capital, on Wednesday 16 October. Thereafter, procedures for the export of the collected soil samples were carried out. Mauritania prohibits the export of desert sand to foreign countries, so that it was necessary to obtain permission from the relevant ministries, such as the Ministry of Mines and the Ministry of Petroleum. The aim of the present study was to establish a method for predicting the spread of mercury-contaminated soil. In addition to getting permission, it was necessary to obtain wind direction and speed data for the area around Chami in order to analyze the dispersion of mercury contamination, a visit was made to the Meteorological Office to obtain relevant information.

In addition, I made two visits before I went back to Japan. The first one is the Japanese embassy in Mauritania (Figure 2), where I collected general information on Mauritania and discussed research collaboration between Japan and Mauritania. The counselor of Japanese embassy told me that the director of national park, PNBA, is really worried about the mercury contamination and is keen to collaborate with me. As a matter of fact, as Chami is located 30 km east of PNBA, there is a risk that mercury contamination spreads to the national park in the future, considering the direction of wind in the region. Hence, we discussed what kind of collaboration can be possible among Japan (Kumamoto University), PNBA agency, and The University of Nouakchott. The second visit is The University of Nouakchott, where I met Prof. Ahmedou MAHFOUDH again to report the result of soil sampling, obtain a letter for exportation, and make a discussion on future collaboration. We concluded that we should keep and foster this collaboration by adding the PNBA agency in order to protect the environment and evaluate the risk of mercury contamination in the future.

Figure 2: Japanese embassy

Figure 3: The University of Nouakchott

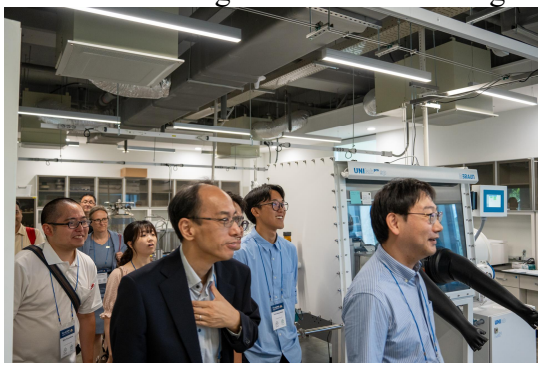
No.3-2-10	Construction of Molecular Spin Qubit Based on External Stimuli Complexes		
Name	Yoshihiro SEKINE	Title	Associate Professor
Affiliation	Priority Organization for Innovation and Excellence Email: sekine@kumamoto-u.ac.jp		
Period of Travel	August 29, 2024 - September 5, 2024		
Visited Researcher	Kil Sik MIN	Title	Professor
Affiliation	Kyungpook National University, Korea		

[Details of activities]

1. Research outline and its perspective

During the stay, we discussed the manuscript construction of international research based on molecular-based magnets.

In addition, I have opportunities to attend the lab tour at the Center for Quantum Nanoscience. That institute is in Seoul, Korea, and specializes in quantum computing observation using STM and fabricating functional nanomagnetic compounds.



2. Research progress and results in the fiscal year

We plan to submit our international studies to the Journal. During our discussion, we realized to synthesis several derivatives and measure physical properties. In the fiscal year, we will conduct it and have finalized the manuscript.

3. Research plan for the next year

Based on this year's results, I plan to prepare new coordination compounds showing characteristic slow magnetic relaxation.

4. List of journal papers published between April 2024 and March 2025.

R. Fukushima, Y. Sekine*, Z. Zhang, S. Hayami*, *J. Am. Chem. Soc.* 2024, 146, 35, 24238–24243 (Supplemental Cover, Kumamoto University Press Release)

5. List of awards, grants, and patents

Kakenhi Kiban C

No.3-2-11	Efficient Molecular Dynamics Simulation Based on Potential Averaging Using Allegro Model		
Name	Kohei SHIMAMURA	Title	Assistant Professor
Affiliation	Faculty of Advanced Science and Technology Email: shimamura@kumamoto-u.ac.jp		
Period of Travel	August 18, 2024 - August 31, 2024		
Visited Researcher	Priya VASHISHTA	Title	Professor
Affiliation	University of Southern California, USA		

[Details of activities]

1. Research outline

We conducted a comprehensive study employing first-principles molecular dynamics (FPMD) simulations and machine-learning interatomic potentials (MLIP). Using non-adiabatic FPMD simulations, we investigated charge transfer rates and the underlying mechanism of the experimentally observed negative resistance in silicon-graphene systems. Additionally, we explored the dissociation dynamics of organosilicon molecules. For MLIP, we focused on thermal conductivity calculations using graph neural network (GNN)-based MLIP. Furthermore, we implemented a potential averaging method to enhance the robustness of MD simulations utilizing GNN-type MLIP.

2. Research progress and results in the fiscal year

[Non-adiabatic FPMD simulations of silicon-graphene system]

This research theme was provided by the team at University of Southern California (USC), and simulations were performed by a student from our laboratory at Kumamoto University. We estimated the charge transfer rates of holes and excited electrons from silicon to graphene and defined the current I from silicon to graphene. Additionally, we derived the voltage V corresponding to the electric field applied to the system. Based on these results, we were able to analyze the I-V relationship for the silicon-graphene system in a manner consistent with experimental findings, where negative resistance was observed. The negative resistance was attributed to the charge transfer rate of holes exceeding that of excited electrons at certain voltages, due to complex band shifts in graphene and silicon induced by external electric fields. The results of this study have been published [i].

[i] H. Hokyo, *et al.*, J. Phys. Chem. Lett, **15**, 9226 (2024).

[Non-adiabatic FPMD simulations for dissociation of organosilicon molecules]

This research theme was also provided by the team at USC, with simulations conducted by students from our laboratory at Kumamoto University. Experimentally, it is known that exposing organosilicon molecules to light can produce SiC nanomaterials. However, it is not well understood whether this process proceeds photochemically or photothermally. Through non-adiabatic FPMD simulations, we found that the dissociation proceeds via a photochemical pathway.

[Thermal conductivity calculation using GNN-type MLIP]

GNN-type MLIPs offer advanced descriptors compared to conventional MLIPs, making them particularly useful for identifying thermoelectric material candidates with low thermal conductivity. While I (Shimamura) have sufficient expertise in thermal conductivity calculations, such as the Green-Kubo method, I lacked experience in programming GNN-type MLIPs. For this reason, I received technical support for GNN-type MLIP programming from the team at USC. Together, we established a method for calculating thermal conductivity using the Allegro model, which is noted for its low computational cost among GNN-type MLIPs. The results of this study have been published [ii].

[ii] K. Shimamura, *et al.*, Int. J. Heat Mass Trans., **234**, 126106 (2024).

[For a robust MD simulation with GNN-type MLIP using potential averaging method]

The potential averaging (PA) method enhances the stability of MD simulations by using the averaged outputs of multiple MLIPs [iii]. Allegro, one of the GNN-type MLIPs, constructs more sophisticated descriptors, and we anticipate that applying the PA method to Allegro could lead to improved accuracy. However, due to the large number of weights in Allegro, applying the PA method without a strategy would result in a significantly high computational cost. To address this, I proposed a method where different weights are introduced in only a specific part of Allegro, while common weights are used for most of the remaining sections. Allegro primarily uses its weights to generate descriptors, and in the final step, it employs a feed-forward NN to convert those descriptors into energy. However, this approach required substantial modifications to the Allegro model, for which technical support from the team at USC was indispensable.

We successfully conducted MD simulations using the PA method using multiple Allegro models. However, the major version update to Pytorch 2.0, which is used to program Allegro, has hindered the implementation of methods designed to reduce computational costs.

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

3. Research plan for the next year

[Non-adiabatic FPMD simulations for dissociation of organosilicon molecules]

We plan to publish the results in papers.

[For a robust MD simulation with GNN-type MLIP using potential averaging method]

We will first implement Allegro to make it compatible with Pytorch 2.0. Next, we will modify the feed forward NN part of Allegro to enable the PA method and reduce computational cost.

4. List of journal papers published between April 2024 and March 2025.

1. Hinata Hokyo, Kai Ito, Rajiv K Kalia, Rehan Kapadia, Aiichiro Nakano, Kohei Shimamura, Fuyuki Shimojo, and Priya Vashishta
   Photoinduced Negative Differential Resistance at a Graphene/Silicon Interface: A Nonadiabatic Quantum Molecular Dynamics Study
   The Journal of Physical Chemistry Letters, Vol. 15, pp. 9226-9232 (2024). DOI: 10.1021/acs.jpclett.4c02272

2. Kohei Shimamura, Shinnosuke Hattori, Ken-ichi Nomura, Akihide Koura, Fuyuki Shimojo
   Thermal conductivity calculation using homogeneous non-equilibrium molecular dynamics simulation with Allegro
   International Journal of Heat and Mass Transfer, Vol. 234, 126106 (8 pp.) (2024). DOI: 10.1016/j.ijheatmasstransfer.2024.126106

5. List of awards, grants, and patents
JSPS KAKENHI Grant Number 22K03454.

No.3-2-12	Development of Machine-Learning Interatomic Potentials and Studies of First-Principles Molecular Dynamics Simulations for Semiconductors		
Name	Kohei SHIMAMURA	Title	Assistant Professor
Affiliation	Faculty of Advanced Science and Technology Email: shimamura@kumamoto-u.ac.jp		
Period of Travel	December 25, 2024 - January 8, 2025		
Visited Researcher	Priya VASHISHTA	Title	Professor
Affiliation	University of Southern California, USA		

[Details of activities]

1. Research outline

We conducted two research projects using first-principles molecular dynamics. The first focused on elucidating the formation process of nano-silicon carbide materials, while the second investigated the diffusion behavior of a tungsten atom on Pt or graphene surfaces. Based on discussions of our research findings in both projects, we plan to publish the simulation results in papers.

Additionally, we have developed a graph neural network-based machine-learning interatomic potential capable of performing robust molecular dynamics simulations. We would also like to publish the results of this development as papers.

2. Research progress and results in the fiscal year

[Non-adiabatic FPMD simulations for dissociation of precursor molecules of nano-SiC]

Silicon carbide (SiC) is a material used in power semiconductors, but it is extremely difficult to process due to its high mechanical strength. Therefore, an approach has been proposed to synthesize nano-SiC semiconductors by utilizing laser-induced decomposition of polymers containing Si and C atoms. However, experimentally elucidating the response mechanism of polymers under laser irradiation poses significant challenges. Since the chemical reactions involved are expected to proceed on the femtosecond and nanometer scales, tracking the movement of individual atoms is quite difficult. The lack of detailed understanding of the response mechanism hinders the rational design of suitable polymer structures.

Under the circumstances, computational simulations based on non-adiabatic first-principles molecular dynamics (NAFPMD) [i], which can handle excited electronic states, provide us with atomic-level insights. This research topic was proposed by the University of Southern California (USC) team. Our research group at Kumamoto University, leveraging its expertise, devised a concrete strategy for NAFPMD simulations, which were then conducted in collaboration with students of the USC team.

We performed NAFPMD simulations on polymer molecular structures designed by experimentalists based on their experience. These simulations revealed that interatomic bonds in proximity to oxygen atoms undergo dissociation. The decomposition of molecular structures was attributed to two possible mechanisms: thermal decomposition due to temperature rise following electronic excitation (i.e., photothermal decomposition) and decomposition induced by carrier effects associated with electronic excitation (i.e., photochemical decomposition). Through detailed analysis, we identified that holes generated near oxygen atoms as a result of electronic excitation caused the dissociation of these interatomic bonds. This finding indicates that the decomposition proceeded photochemically. Since there are numerous candidate molecular structures, we plan to repeat this simulation

procedure to elucidate the atomic-level mechanisms and accumulate knowledge for the rational design of polymer molecular structures.
[i] F. Shimojo, *et al.*, Comput. Phys. Commun. **184**, 126106 (2013).

[FP calculations for diffusion of tungsten atom on Pt/Graphene surfaces]

Pt surfaces are commonly used for engineering applications. However, the mobility of tungsten atoms on these surfaces is not well understood. If the mobility is low, tungsten atoms may cluster, potentially degrading the performance of devices on Pt surfaces. Incidentally, replacing Pt surfaces with graphene has been proposed as a way to improve the device performance based on experimental results. However, the reason why graphene is superior is not yet understood. We thus investigate the mobility of tungsten atoms between stable sites on Pt and graphene surfaces from the perspective of adsorption and activation energies using first-principles (FP) calculations. This research topic was also provided by the USC team. Members of our laboratory at Kumamoto University proposed a specific strategy for FP calculations, and the calculations were performed by our students. We found that the adsorption energy is higher on the Pt surface, meaning that it is more difficult to desorb tungsten atoms from Pt than from graphene. On the other hand, the activation energy for mobility between stable sites is currently under calculation.

[Application of potential averaging method to machine-learning interatomic potentials]

We have retuned the Allegro model [ii], which is one of the graph neural network-type machine-learning interatomic potentials (MLIPs). Recently, significant updates were made to the Allegro model due to a major version update of the underlying Pytorch library and a transition to the Pytorch Lightning environment, which has enhanced versatile implementation of models. We applied the potential averaging (PA) method [iii] to this new version of the Allegro model. The PA method improves the stability of MD simulations by using averaged outputs from multiple MLIPs. We have been already validating the effectiveness of the PA method using different type MLIPs and have confirmed its substantial effectiveness in stabilizing the simulations [iii]. Furthermore, by using the PA method, we can also assess the errors associated with the averaged output. A large error indicates insufficient training of models, which provides an opportunity to gather new training data for retraining the MLIP to enhance its robustness.
[ii] A. Musaelian, *et al.*, Nat. Commun., **14**, 579 (2023).
[iii] D. Wakabayashi, *et al.*, J. Phys. Soc. Jpn., **92**, 054005 (2023).

3. Research plan for the next year

[Non-adiabatic FPMD simulations for dissociation of precursor molecules of nano-SiC]

We plan to publish the results in papers.

[FP calculations for diffusion of tungsten atom on Pt/Graphene surfaces]

We plan to publish the results in papers.

[Application of potential averaging method to machine-learning interatomic potentials]

Recently, MLIPs trained on data from compounds composed of the majority of elements in the periodic table have emerged, known as Foundation Models (FM). Users can utilize FM whenever and, if necessary, perform fine-tuning to improve accuracy. This approach differs significantly from the traditional method, where MLIPs were constructed over time for each specific material. With the introduction of the PA method, the fine-tuning becomes easier by utilizing the errors in the outputs. We are currently preparing a paper on this implementation, with a focus on applying it to FM.

4. List of journal papers published between April 2024 and March 2025.

1. Hinata Hokyo, Kai Ito, Rajiv K Kalia, Rehan Kapadia, Aiichiro Nakano, Kohei Shimamura, Fuyuki Shimojo, and Priya Vashishta
   Photoinduced Negative Differential Resistance at a Graphene/Silicon Interface: A Nonadiabatic Quantum Molecular Dynamics Study
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   DOI: 10.1021/acs.jpclett.4c02272

2. Kohei Shimamura, Shinnosuke Hattori, Ken-ichi Nomura, Akihide Koura, Fuyuki Shimojo
   Thermal conductivity calculation using homogeneous non-equilibrium molecular dynamics simulation with Allegro
   International Journal of Heat and Mass Transfer, Vol. 234, 126106 (8 pp.) (2024).
   DOI: 10.1016/j.ijheatmasstransfer.2024.126106

5. List of grants

JSPS KAKENHI Grant Number 22K03454.

No.3-2-13	Development of Wearable Ultrasound Sensors for Next-Generation Healthcare		
Name	Masayuki TANABE	Title	Assistant Professor
Affiliation	Faculty of Advanced Science and Technology Email: mtanabe@cs.kumamoto-u.ac.jp		
Period of Travel	December 10, 2024 - December 20, 2024		
Visited Researcher	Prabal Datta BARUA	Title	Professor
Affiliation	University of Southern Queensland, Australia		

[Details of activities]

1. Research Outline and Perspective

This research aims to apply ultrasonic sensing technology to the medical field by using wearable sensors for real-time physiological monitoring. We focus on device wearability, measurement accuracy, and the development of data analysis methods, with applications in telemedicine and home care in mind. Through this visit, we plan to strengthen collaboration among team members, establishing a sustainable, interdisciplinary research framework.

2. Research Progress and Results in the Current Fiscal Year

Demonstrated the wearable ultrasonic sensor developed at Kumamoto University in Sydney, Australia, confirming its feasibility in terms of wearability and measurement accuracy, while identifying technical challenges.

Collaborated with the local team to outline practical implementation procedures and a roadmap for commercialization in the medical sector, thereby laying the groundwork for international joint research.

Established a continuous research framework by confirming that one team member will enroll in the doctoral program at Kumamoto University from Australia.

3. Research Plan for the Next Year

Aim to further enhance the performance of the wearable ultrasonic sensor and expand its potential applications by upgrading the device and testing prototypes.

Introduce advanced data analysis methods (AI, machine learning, etc.) to fully leverage measurement data and explore possibilities for telemedicine and home care.
Reschedule discussions with the Brisbane-based research team to accelerate international collaborative research efforts.

4. List of Journal Papers Published or Planned for Publication Between April 2024 and March 2025

Currently preparing a manuscript. We plan to present at conferences and submit for publication within 2025.

5. List of Awards, Grants, and Patents

None.