3-2. IROAST International Joint Research Travel Support Program

No.	Name	Destinations / Period
3-2-1	**Jonas Karl Christopher Nuevas AGUTAYA** IROAST	University of Tübingen (Germany) March 4, 2023 - March 19, 2023
3-2-2	**Hamid HOSANO** IINa	Imperial College London (UK) August 15, 2022 - August 26, 2022
3-2-3	**Hamid HOSANO** IINa	1) The University of Glasgow (UK) 2) Imperial College London (UK) February 20, 2023 - March 3, 2023
3-2-4	**Makiko KOBAYASHI** FAST **Masayuki TANABE** FAST	Ngee Ann Polytechnique Singapore (Singapore) December 11, 2022 - December 14, 2022
3-2-5	**Nobutatsu MOCHIZUKI** FAST	1) The University of Orléans and Laboratoire Magmas et Volcans (France) 2) The University of Clermont Auvergne (France) September 26, 2022 - October 6, 2022
3-2-6	**Ruda LEE** IINa	Korea Basic Science Institute (Korea) August 17, 2022 - August 31, 2022
3-2-7	**Ruda LEE** IINa	1) Korea Basic Science Institute (Korea) 2) Kangwon National University (Korea) February 24, 2023 - March 5, 2023
3-2-8	**Yoshihiro SEKINE** POIE	Institut Kimia Malaysia (Malaysia) November 21, 2022 - November 25, 2022
3-2-9	**Kohei SHIMAMURA** FAST	University of Southern California (USA) December 26, 2022 - January. 08, 2023

FAST：Faculty of Advanced Science and Technology

IINa：Institute of Industrial Nanomaterials

POIE：Priority Organization for Innovation and Excellence

Report on IROAST International Joint Research Travel Support Program

No. 2-1	Elucidation of the gas sensing mechanism of semiconductor metal oxides from *operando* DRIFTS measurements		
Name	Jonas Karl Christopher Nuevas AGUTAYA	Title	Postdoctoral fellow
Affiliation	IROAST (Kida Laboratory) Email: jnagutaya@chem.kumamoto-u.ac.jp		
Period of Travel	March 4, 2023- March 19, 2023		
Visited Researcher	Nicolae BARSAN	Title	Group Head
Affiliation	Weimar Group, Institute of Physical and Theoretical Chemistry University of Tübingen (Germany)		

[Details of activities]

1. Research outline and its perspective

   Understanding the science behind the detection mechanism of gas sensors paves the way for the improvement of their performance and the design of better devices. In this field, DRIFTS has become an invaluable tool because it allows for the identification of the analytes that are adsorbed on the surface of the sensing materials, such as semiconductor metal oxides. Furthermore, by employing *operado* DRIFTS, the changes that the adsorbed species undergo can be monitored under their controlled or actual detection conditions.

2. Research progress and results in the fiscal year

   With respect to this project, any measurements using DRIFTS has not been performed. In the previous fiscal year, the primary focus was theoretical calculations, specifically the charge density difference, density of states, and surface reaction mechanism. These types of calculations complement the results of DRIFTS measurements to provide a comprehensive elucidation of the gas sensing mechanism of semiconductor metal oxides, the sensing material in this study.

3. Research plan for the next year

   Using the DRIFTS apparatus available in the laboratory, the performance of pristine and surface-modified ZnO and SnO_2 in the detection of gases such as ethanol, acetone, and carbon monoxide will be evaluated. Theoretical calculations using DFT will also be performed to reinforce the experimental results.

4. List of journal papers

   - Kam, Y. L.; Agutaya, J. K. C. N.; Quitain, A. T.; Ogasawara, Y.; Sasaki, M.; Lam, M. K.; Yusup, S.; Assabumrungrat, S.; Kida, T. “In-Situ Transesterification of Microalgae Using Carbon-Based Catalyst under Pulsed Microwave Irradiation”. Biomass and Bioenergy 2023, 168. https://doi.org/10.1016/J.BIOMBIOE.2022.106662.

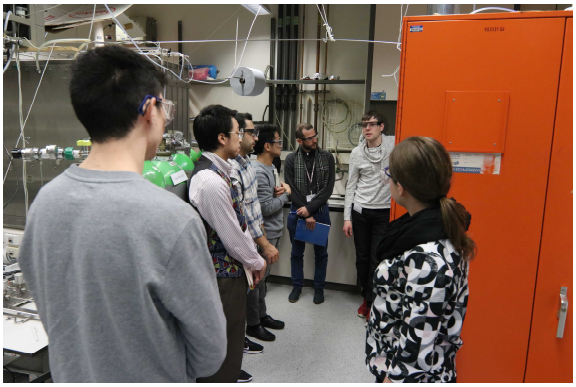
5. List of awards, grants, and patents, if any

   - Best Poster Presentation Award at the 48th International Congress on Science, Technology and Technology-Based Innovation (Thailand, Nov. 29–Dec. 1, 2022) for the study titled “Theoretical study of the formation of hydroxyl groups on Pt-doped

ZnO(10-10) from the heterolysis of water”

Photos from the trip

Discussion of the theory behind the Kelvin probe



Demonstration of the use of the Kelvin probe

Visit to the Lichtenshtein castle

Report on IROAST International Joint Research Travel Support Program

No. 2-2	Novel efficient and green protein/hydrocarbon extraction from microalgae		
Name	Hamid HOSANO	Title	Professor
Affiliation	Institute of Industrial Nanomaterials (IINa) Email: hamid@kumamoto-u.ac.jp		
Period of Travel	August 15, 2022 – August 26, 2022		
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 10 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 work on efficient oil and protein extractions from microalgae and study protein 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.

2. Research achievements and progress of the international joint research

A joint research was performed to work on simulation of protein nanoparticle formation from industrial waste. Prof. Rigopoulos and his Ph.D. student will work on population balance modelling and Hosano and his collaborators will provide experimental evidences. In this respect a joint journal manuscript was initiated. We also discussed to collaborate on efficient oil and protein extraction from microalgae. This CO_2 capturing project is of Kumamoto University's interest, which refers to 2nd and 7th SDGs goals.
To achieve our goals of these multidisciplinary subjects, we have mobilized a team with complementary expertise for the project.

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

Discussions and lab visits were performed at Prof. Rigopoulos's laboratories to facilitate the joint research and collaboration. Prospects and required simulations in the ME Department, ICL, and experiments in the IINa, Kumamoto University, were discussed and arranged. The collaboration program and the joint journal manuscript will be followed up during future visits.

Comments or suggestions for IROAST (programs)
We would like to acknowledge and thank the support of IROAST to facilitate the visit and to make the collaboration to be possible.
The IROAST programs play a key role in providing opportunity to Kumamoto University's young and research faculties to extend their experiences/knowledge through collaboration with world

renowned groups.

Meeting Prof. RIGOPOULOS, Department of Mechanical Engineering, Imperial College London.

Working discussion and project management with Prof. RIGOPOULOS and his Ph.D. student, Department of Mechanical Engineering, Imperial College London.

Report on IROAST International Joint Research Travel Support Program

No. 2-3	Vortex ring formation following shock wave diffraction / keratin nanoparticles derived from industrial feather waste		
Name	Hamid HOSANO	Title	Professor
Affiliation	Institute of Industrial Nanomaterials (IINa) Email: hamid@kumamoto-u.ac.jp		
Period of Travel	February 20, 2023 – March 3, 2023		
Visited Researchers	Konstantinos KONTIS	Titles	Professor-Dean
Affiliations	The University of Glasgow, UK		
Visited Researchers	Stelios RIGOPOULOS Mazdak GHAJARI	Titles	Reader Senior Lecturer
Affiliations	Imperial College London, UK		

1. Overview and significance of the international research collaboration

The University of Glasgow (UoG) is ranked 81st in the QS World University and 82nd in Times Higher Education (Elsevier) Rankings; it is the fourth-oldest university in the English-speaking world. Prof. Kontis is the Dean of Global Engagement; during the visit connecting Graduate Schools of the University of Glasgow and Kumamoto University has been discussed and arranged. Specific research collaboration regarding vortex ring formation following shock wave diffraction has been performed.
The Imperial College London (ICL) is ranked 6th in the QS and 10th in the Times Higher Education (Elsevier) World University Rankings. ICL is a public research university with 14 Nobel laureates, 87 Fellows of the Royal Academy of Engineering, and 85 Fellows of the Academy of Medical Sciences. The ICL has several world leading centers including Department of Brain Sciences and Nanomaterials (Department of Mechanical Engineering), very appropriate for joint research with IROAST and Kumamoto University. The green hydrocarbon/protein extractions and nanoparticle formation form industrial waste joint projects with Prof. Rigopoulos have been of great interest. Collaboration with Prof. Ghajari for traumatic brain injuries has been important to understand the mechanisms and consider appropriate prevention methods. Experiments in this respect are underway with the Neurosurgeon colleagues.

2. Research achievements and progress of the international joint research

High pressure gas from thrusters of a satellite or a spacecraft has the potential to experience shock wave diffraction and the formation of compressible vortex rings. Understanding this transient phenomenon is important for improving the thrust vector and avoiding surface contamination. However, limited transient experimental results of compressible vortex rings in low-pressure environments can be found. Prof. Kontis and Hosano have been conducting joint research to study compressible vortex rings in reduced pressure environments, the visit facilitated a joint publication in this regard.
The visit also served to follow up with Prof. Rigopoulos regarding a joint research we started during Hosano's previous visit. We started to prepare a manuscript for publication regarding population balance modelling and computational fluid dynamics simulations of keratin protein nanoparticle formation. Chicken slaughterhouses produce extensive waste, mainly feathers, that needs to be managed properly to prevent environmental pollution. Low cost, biodegradability, low immunogenicity, and colloidal stability of recycled feather keratin makes it attractive to produce protein-based nanomaterials. This waste recycling project has been of Kumamoto University's

interest and refers to 2nd and 7th SDGs goals.
Prof. Ghajari and Hosano have been planning to organize a “Brain Injuries” session during “the World Congress of the International Society of Medical Shockwave Treatment ISMST” following “the 34th International Symposium on Shock Waves ISSW34”. During the visit they met and arranged the session. Further visits and collaborations were planned.

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

Discussions and lab visits were performed at Prof. Kontis and Prof. Rigopoulos laboratories to facilitate the joint researches and collaborations. Prospects and required experimental devices and simulation facilities in the UoG and ICL, and experiments in the IINa, Kumamoto University, were discussed and arranged. The collaboration programs and the further joint journal articles will be followed up during future visits. We planned for UK-Japan grant applications to financially support the joint researches. Specifically, we aim for applying for JSPS Bilateral Joint Research Projects.

Meeting Prof. Kontis at the University of Glasgow.

Discussion with Prof. Kontis at the School of Engineering, the University of Glasgow.

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

Meeting with Prof. Ghajari at the Dyson School of Design Engineering, Imperial College London.

Report on IROAST International Joint Research Travel Support Program

No. 2-4	Advanced Biomedical Evaluation System		
Name	Makiko KOBAYASHI	Title	Professor
Affiliation	Faculty of Advanced Science and Technology (FAST) Email: kobayashi@cs.kumamoto-u.ac.jp		
Name	Masayuki TANABE	Title	Assistant Professor
Affiliation	Faculty of Advanced Science and Technology (FAST) Email: mtanabe@cs.kumamoto-u.ac.jp		
Period of Travel	December 11, 2022-December 14, 2022		
Visited Researcher	Rajendra Udyavara ACHARYA Ru San TAN	Title	Senior Faculty member Senior Consultant
Affiliation	Ngee Ann Polytechnique Singapore, Singapore		

[Details of activities]
The goal of this research is to develop a flexible ultrasonic sensor for medical use. The wearable ultrasonic sensor, developed using a sol-gel composite spray technique, aims to enable long-term monitoring of the heart and arm blood vessels. The research focuses on detecting and predicting myocardial infarction and monitoring blood pressure in real-time.

During this year's study, we successfully produced a prototype ultrasonic sensing system in Japan. The preliminary experiment, conducted under the guidance of Dr. Tan Ru San, a cardiologist at National Heart Center Singapore, was also successful. The results showed the potential of the ultrasonic sensor in monitoring blood pressure in real-time.

Moving forward, we plan to conduct clinical trials to further validate the effectiveness of our ultrasonic sensor in detecting and predicting myocardial infarction and monitoring blood pressure. We believe that the ultrasonic sensor has great potential in revolutionizing the field of medical sensing, making healthcare more accessible and convenient for people in need.

[Journals]
Masayuki Tanabe and Kosuke Sato and Toru Uda and Makiko Kobayashi. Thin, flexible, and biocompatible medical ultrasound array transducer using a sol–gel composite spray technique, Japanese Journal of Applied Physics, Vol. 62, 2023, pp. SJ1034,
doi: 10.35848/1347-4065/acbc27.

Report on IROAST International Joint Research Travel Support Program

No. 2-5	Paleointensity study of the Laschamp geomagnetic excursion		
Name	Nobutatsu MOCHIZUKI	Title	Associate Professor
Affiliation	Faculty of Advanced Science and Technology (FAST) Email: mochizuki@kumamoto-u.ac.jp		
Period of Travel	September 26, 2022- October 6, 2022		
Visited Researcher	Kenneth KOGA	Title	Professor
Affiliation	The University of Orléans and Laboratoire Magmas et Volcans, France		
Visited Researcher	Geeth MANTHILAKE	Title	Researcher
Affiliation	The University of Clermont Auvergne, France		

[Details of activities]

1. Research outline and its perspective

   The Laschamp geomagnetic excursion, occurred at 40,000 years ago, has been recorded by remanent magnetization of lava flows of multiple volcanoes in Massif Central, France. During this excursion, the geomagnetic field intensity showed a significant decrease by a factor of 5 or more as well as a large deviation of more than 90 ° from the axial dipole field direction. In order to recover the geomagnetic field vector behavior during the excursion, we made a field survey to collect rock samples from the lava flows which record the Laschamp excursion and the geomagnetic fields just before/after the excursion.

   Fig. 1. Sampling at a lava flow of Volvic volcano in Massif Central (left photograph). Rock samples were oriented by using the three-point orientation tool with a magnetic compass (right photograph).

2. Research progress and results in the fiscal year

   During the period between September 26, 2022 and October 6, 2022, we visited Laboratoire Magmas et Volcans, The University of Clermont Auvergne and made a field survey at volcanoes in Massif Central. First of all, we had a meeting with Prof. Kenneth Koga and Dr. Geeth Manthilake for promoting this research project and future possible collaborations. They also gave us important information for our field survey to collect volcanic rocks of volcanoes in Massif Central. During our field survey, we visited eight sites (locations) at six lava flows of volcanoes in Massif Central. At the eight sites, we sampled 86 block samples, which were oriented by the three-point orientation tool with a Brunton magnetic compass (see Fig. 1).

After the travel, we started pilot paleointensity measurements on the collected samples in the paleomagnetic laboratory in Kumamoto University. Both the Thellier-type and Shaw-type paleointensity methods were applied to some samples from the Laschamp and Royat lava flows. The pilot experiments of Shaw-type paleointensity method are successful, which gave very weak paleointensities of 6-11 micro T. We also started rock-magnetic measurements of thermomagnetic analyses on the samples (Fig. 2) in order to investigate magnetic properties which may be linked to successful/failed paleointensity results.

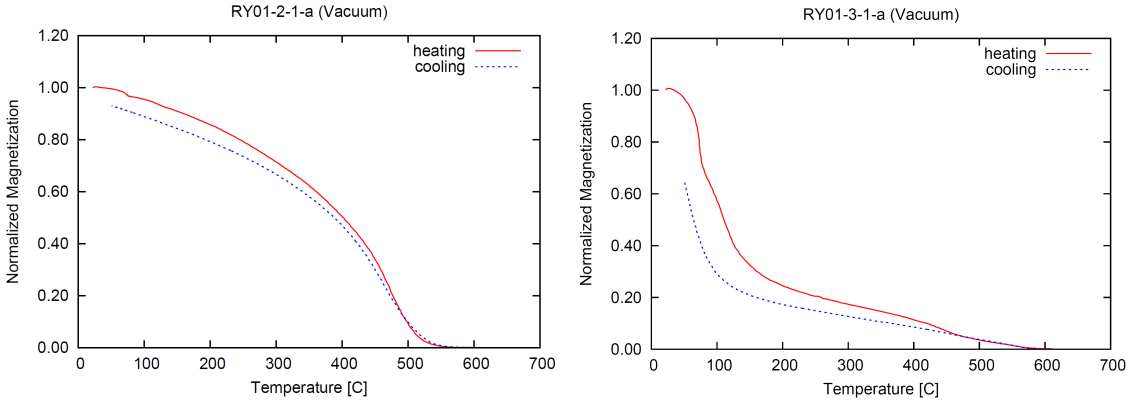


Fig. 2. Thermomagnetic curves for the samples from Royat lava (site RY01). A single Curie temperature of ~500 °C, corresponds to titanium-poor titanomagnetite, is recognized in the sample of RY01-2 (left). Two Curie temperature phases of ~150 °C and 500-600 °C, which correspond to titanium-rich and titanium-poor titanomagnetite, respectively, are recognized in the sample of RY01-3 (right).

3. Research plan for the next year

We are going to make paleointensity measurements on several samples from the eight sites for six lava flows. We will obtain three or more paleointensity values for each site and then calculate an average of them. These averages will be new reliable paleointensity estimates for the Laschamp geomagnetic excursion. At the end of this year, my graduate student will write a master thesis on this research topic (in Japanese). We will also start to write a draft (in English) for publication in an international journal.

4. List of journal papers (with IROAST as your affiliation) published between April 2022 and March 2023.

(none)

5. List of awards, grants, and patents, if any

(none)

Report on IROAST International Joint Research Travel Support Program

No. 2-6	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 Nano Materials (IINa) Email: aeju-lee@kumamoto-u.ac.jp		
Period of Travel	August 17, 2022-August 31, 2022		
Visited Researcher	Seung-Hae KWON	Title	Principal Investigator
Affiliation	Korea Basic Science Institute, Korea		

[Details of activities]

1. Research outline and its perspective

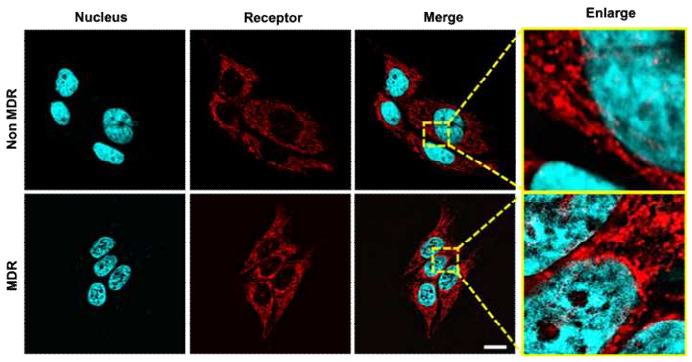
A better understanding of the underlying molecular interactions of receptor-multidrug resistance (MDR)-immune cells in 3D environment is required to develop successful therapeutic strategies to overcome MDR. Live cell imaging of the MDR mechanism is less prone to experimental artifacts and can provide 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

We investigated six different triple-negative breast cancer cell lines and found one typical pattern in receptor expression after obtaining the drug resistance characteristics. That is one of the receptors overexpressed in MDR cells compared to non-MDR cells. We modified nanoparticles with the receptor target ligand based on this finding. Now, we've got positive results showing a higher cell accumulation rate.

3. Research plan for FY2023

Currently, we are focusing on quantifying the number of receptors. The data will be analyzed by imaging software and categorized. In September 2023, six TNBC cell receptor translocations will confirm that the high-resolution images and organized with MDR overcoming nanoparticles. This finding has to be confirmed by a mechanism study, so I will discuss it with a biologist at Max Planck Institute Munich.



Report on IROAST International Joint Research Travel Support Program

No. 2-7	Overcoming multidrug resistance in breast cancer with topoisomerase inhibitor loaded polymersome		
Name	Ruda LEE	Title	Associate Professor
Affiliation	Institute of Industrial Nano Materials (IINa) Email: aeju-lee@kumamoto-u.ac.jp		
Period of Travel	February 24, 2023-March 5, 2023		
Visited Researcher	1) Sang Hee NAH 2) Jung Hoon CHOI	Title	Principle Investigator
Affiliation	1) Korea Basic Science Institute, Korea 2) Kangwon National University, Korea		

[Details of activities]

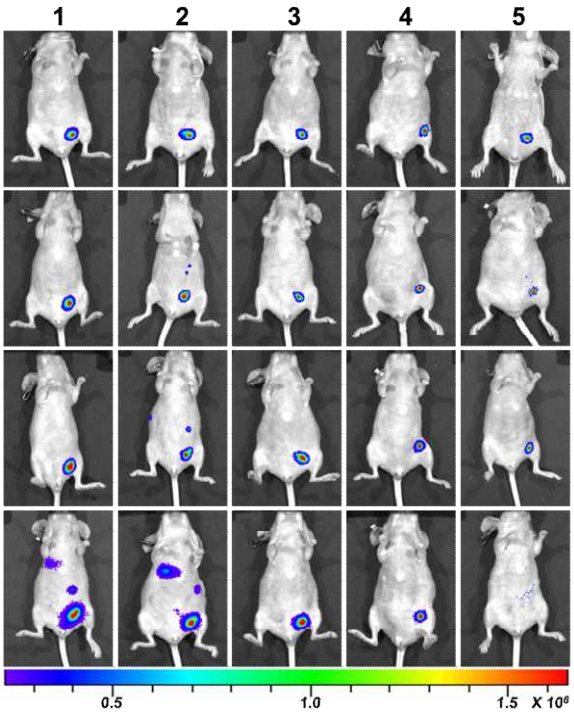
1. Research outline and its perspective

Numerous treatment strategies are being developed, including innovative biological treatments for specific cellular pathways. However, the inherent multidrug resistance (MDR) to chemotherapy drugs remains a significant obstacle to effective breast cancer treatment.

This research aims to confirm the efficacy of Lee lab-developed NPs against acquired and innate drug-resistance breast cancer cells and evaluate in vivo.

2. Research progress and results

We finalized the MDR animal model experiment and analysis. As we expected, Lee lab developed NPs showing the highest MDR tumor overcoming effect and inhibiting the metastasis.



3. Research plan for FY2023

Currently, we are focusing on analyzing the tumor species. At the same time, I'm preparing a manuscript for Biomaterials (IF 15.304). We are expecting to submit the paper in May.

Report on IROAST International Joint Research Travel Support Program

No. 2-8	Development of external-stimuli-responsive molecular compounds		
Name	Yoshihiro SEKINE	Title	Associate Professor
Affiliation	Priority Organization for Innovation and Excellence (POIE) Email: sekine@kumamoto-u.ac.jp		
Period of Travel	November 21, 2022-November 25, 2022		
Visited Event	International Congress on Pure & Applied Chemistry (ICPAC) Kota Kinabalu 2022	Title	—
Organization	Institut Kimia Malaysia (IKM), Malaysia		

Please include the following 1-3:

1. Overview and significance of the international research collaboration

Using this support program, I joined the international conference of "ICPAC Kota Kinabalu 2022" as an invited speaker. It has several parallel scientific sections, and I have mainly attended the "Coordination Chemistry" section to obtain information on scientific topics and trends, and do a discussion about my research topics of "Development of external-stimuli-responsive molecular compounds". For example, I have discussed with Dr. Ryohei, Oka from Nagoya Institute of Technology, and Prof. Wan Mohd Khairul Wan Mohamed Zin from Universiti Malaysia Terengganu, about their research.

2. Research achievements and progress of the international joint research
(co-authored papers if any.)

After my presentation in the thematic section "Inorganic and Coordination Chemistry", I obtained several valuable comments and questions from participants. I also got several information and useful discussion.

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

To the development of external-stimuli-responsive molecular compounds is one of the fundamental and attractive fields of chemistry. For further research progress including international collaboration, this conference was useful for me to make international researcher friends, and have several discussions about my research.

Report on IROAST International Joint Research Travel Support Program

No. 2-9	Study of Hydrogen-Induced Electrical Properties Using First-Principles Molecular Dynamics Simulations and Machine-Learning Interatomic Potentials		
Name	Kohei SHIMAMURA	Title	Assistant professor
Affiliation	Faculty of Advanced Science and Technology (FAST) Email: shimamura@kumamoto-u.ac.jp		
Period of Travel	December 26, 2022 - January 08, 2023		
Visited Researcher	Priya VASHISHTA	Title	Professor
Affiliation	University of Southern California (USA)		

[Details of activities]

1. Research outline

We conducted researches using first-principles molecular dynamics (FPMD) simulations and using machine-learning interatomic potentials (MLIPs). FPMD simulations are used to investigate the mobility of electrons in impurity levels in hydrogen-doped WO_3. For MLIPs, the development of GNN-type and training methods using regularization schemes were discussed. The GNN-type would be applicable to various materials. The regularization schemes have the potential to improve upon the current standard training method. Using such MLIPs, we estimate dielectric functions of water and ammonia.

2. Research progress and results in the fiscal year

[FPMD simulations of hydrogen-doped WO_3]

It was experimentally demonstrated that WO_3, an insulator, can switch the electric current on and off by changing the amount of doped hydrogens [i]. It was assumed that the electric current is generated by the diffusion of electrons in impurity levels created near the conduction band by the doped hydrogens, and by the hydrogen (protons) themselves. To verify this, we created models with different amounts of doped hydrogens and began to investigate them from a microscopic point of view by means of FPMD simulations.

[i] X. Yao, *et al.*, Nat. Commun., **11**, 3134 (2020).

[Applications of GNN-type MLIPs]

We focus on the recently proposed Allegro model [ii]. This MLIP uses descriptors that are quite reasonable from a physical point of view, with Euclidean group (translation, rotation, and mirror-image reversal) equivariance. Therefore, a highly accurate MLIPs can be constructed even with a small number of training data. We plan to construct Allegro for water and ammonia and investigate their physical properties.

[MLIP training methods using regularization]

In previous MLIP training methods, it has been believed that minimizing the training error for diverse training data lead to high accuracy of MLIPs. However, it has become clear that this is not always the case [iii]. Even though the training error is small, the actual physical accuracy may be low. Therefore, excluding the implication, we have begun to develop a training method that imposes important constraints in terms of physics and machine learning by the form of regularization. One is the heat flux regularization (HFR) [iv]. Heat flux is an important physical quantity that reflects energy transport in materials, but it is difficult to set as a training target for MLIPs. The value of heat flux is indefinite because it depends on the initial conditions of the MLIPs such as weight parameters. This is solved by the regularization. The other is Sharpness-Aware Minimization (SAM) [v]. This approach is

expected to improve the generalization performance of MLIPs.
[iii] X. Fu, *et al.*, arXiv:2210.07237 (2022).
[iv] K. Shimamura, *et al.*, arXiv:2204.01405 (2022).
[v] P. Foret, *et al.*, arXiv:2010.01412 (2021).

3. Research plan for the next year

[FPMD simulations of hydrogen-doped WO_3]

Depending on the amount of doped hydrogens, the electrons in the impurity levels are expected to be localized and delocalized. Thus, we will attempt to visualize the dynamics of electrons in a manner by adapting the direct visualization method of electrons that we have used in our previous study [vi]. We also define the center of mass of the electrons and calculate the mean square displacement with respect to the center of mass to quantitatively discuss whether they behave locally or nonlocally.

[vi] T. Hakamata, *et al.*, Sci. Rep., **5**, 19599 (2016).

[Applications of GNN-type MLIPs and training methods using regularization]

For the water and ammonia, we are interested in their dielectric functions. The atomic interactions in these materials are quite complicated and their reproduction requires a high precision of MLIPs. We will examine how the dielectric function estimated in our previous study [vii] differs from the one using Allegro model. In addition, training schemes that take into account the use of the regularization schemes such as HFR and SAM can improve accuracy from both physical and machine learning perspectives.

[vii] A. Krishnamoorthy, *et al.*, Phys. Rev. Letts., **126**, 216403 (2021).

4. List of journal papers

1. A. Krishnamoorthy, *et al.*, J. Phys. Chem. Letts., **13**, 7051 (2022).
2. T. Linker, *et al.*, Front. nanotechnol., **4**, 884149 (2022).
3. M. Misawa, *et al.*, Sci. Rep., 12, 19458 (2022).
4. T. Linker, *et al.*, J. Phys. Chem. Letts., **13**, 11335 (2022).

5. List of grants

1. JSPS KAKENHI Grant Number 22K03454.