## 2-5. Research Clusters

| No. | Name | Project Title |
|---|---|---|
| 2-5-1 | **Hiroki MATSUO**<br>IROAST | Ferroelectric Photovoltaics |
| 2-5-2 | **Gaochuang CAI**<br>IROAST | Next-Generation Design of Structures |
| 2-5-3 | **Masahiko FURUTANI**<br>IROAST | Control of Plant-parasitic Nematodes |
| 2-5-4 | **Zhongyue ZHANG**<br>IROAST | Low-Dimensional Molecular Electronics and Spintronics |
| 2-5-5 | **Shinya HAYAMI**<br>FAST | Development of Nano and Supramolecular Materials |
| 2-5-6 | **Sinichiro SAWA**<br>FAST | Plant Cell and Developmental Biology |
| 2-5-7 | **Makoto TAKAFUJI**<br>FAST | Nano-Organics and Nano-Hybrids |
| 2-5-8 | **Hamid HOSANO**<br>IINa | Nano-medicine and Drug Delivery System |
| 2-5-9 | **Takuro NIIDOME**<br>FAST | Nano-medicine and Theranostics |
| 2-5-10 | **Toshifumi MUKUNOKI**<br>FAST | Quantification of Three Dimensional Vascular Network |
| 2-5-11 | **Yoji MINE**<br>FAST | Advanced Structural Materials |
| 2-5-12 | **Sadahiro TSUREKAWA**<br>FAST | Microstructure Analysis and Grain Boundary Engineering |
| 2-5-13 | **Ichiro AKAI**<br>IINa | Structure and Dynamics of Materials Using Quantum Beams and Data-Driven Sciences |
| 2-5-14 | **Tetsuya KIDA**<br>FAST | Nano-materials for Energy Applications and Environmental Protection |
| 2-5-15 | **Mitsuhiro AIDA**<br>FAST | Plant Stem Cells and Regeneration |

FAST：Faculty of Advanced Science and Technology

IINa ：Institute of Industrial Nanomaterials

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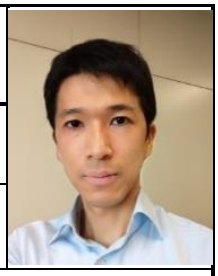
|---|---|---|---|
| No. 2-5-1 | Ferroelectric Photovoltaics | |  |
| **Cluster Coordinator** | | | |
| Name | Hiroki MATSUO | | |
| Affiliation,<br>E-mail | IROAST<br>Email: matsuo_h@cs.kumamoto-u.ac.jp | Title | Associate Professor |
| Research Field | Advanced materials | | |
| **Cluster Members** | | | |
| Name | Affiliation/Title | | |
| Yuji NOGUCHI | Kumamoto University / Professor | | |
| Daisuke KOSUMI | Kumamoto University / Associate Professor | | |
| Ho-Yong LEE | Ceracomp Co. Ltd. / Professor, President | | |
| Moon-Chan KIM | Ceracomp Co. Ltd. / Researcher | | |

## 1. Research outline and its perspective

Ferroelectric materials with spontaneous polarization ($P_s$) exhibit a characteristic photovoltaic (PV) response that does not appear in the pn junctions of conventional semiconductors. High photovoltages, light-polarization-dependent photocurrents, and fast photoresponse are appealing features of the ferroelectric PV effect. We investigate the impact of chemical doping on the PV response of ferroelectric oxides. In this fiscal year, photocarrier dynamics in Mn-doped $BaTiO_3$ single crystals were investigated by using transient absorption spectroscopy (TAS)

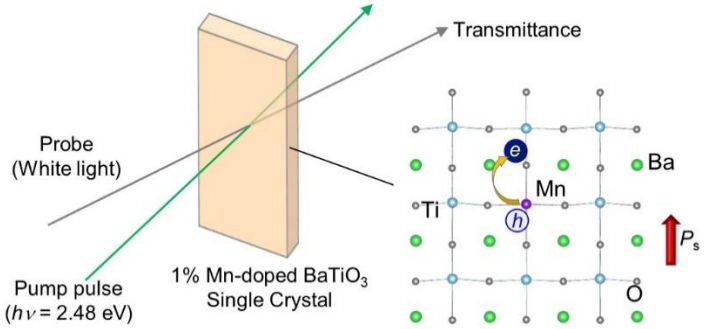



Fig. 1. TAS measurement for Mn-doped $BaTiO_3$ single crystals.

## 2. Research progress and results

The PV properties of 1% Mn-$BaTiO_3$ ($BaTi_{0.99}Mn_{0.01}O_{3-\delta}$) single crystals grown by the solid-state crystal growth method were investigated. The crystals were annealed at 900 °C under a reduced atmosphere to control the valance state of Mn. A poling treatment was performed by applying an external electric field in the <101> direction prior to the PV measurements. TAS measurements were performed for unpoled single crystals after optical polishing.

The photon energy ($h\nu$) dependence of photocurrents in the <101> direction revealed that the Mn-doped single crystals exhibit photocurrent even at $h\nu$ smaller than $E_g$ of $BaTiO_3$ (3.2 eV).

The sample with a mixed valance state of $Mn^{2+}$ and $Mn^{3+}$ showed a larger photocurrent than that with $Mn^{4+}$ and with $Mn^{3+}$. The maximum $I_{sc}/I_{inc}$ ($I_{sc}$: short-circuit photocurrent, $I_{inc}$: incident light intensity) of $4.6 \times 10^{-9}$ $V^{-1}$ $cm^2$ was observed at $h\nu = 2.7$ eV for the sample with $Mn^{2+,3+}$ which is about 7 and 6 times as large as that of the samples with $Mn^{4+}$ and with $Mn^{3+}$, respectively. The $I_{sc}$ measurements for the positively poled and negatively poled samples presented that the direction of the photocurrent changes depending on the polarization direction, which demonstrates that the observed PV response arises from the ferroelectric PV effect.

In the absorption change ($\Delta\alpha$) as a function of the wavelength of probe light ($\lambda_{probe}$) for the $Mn^{2+,3+}$ sample induced by the pump pulse at 2.48 eV ($< E_g$), three broad light-induced absorption bands were observed at $\lambda_{probe}$ of 500 nm–600 nm, 750 nm–850 nm, and 650 nm–750 nm, respectively. In contrast, apparent changes in the absorption were not induced by the pump pulse for undoped $BaTiO_3$ single crystals. This result strongly indicates that the photocarriers are generated by the below-bandgap excitation as a result of the formation of the impurity levels derived from Mn-3d orbitals.

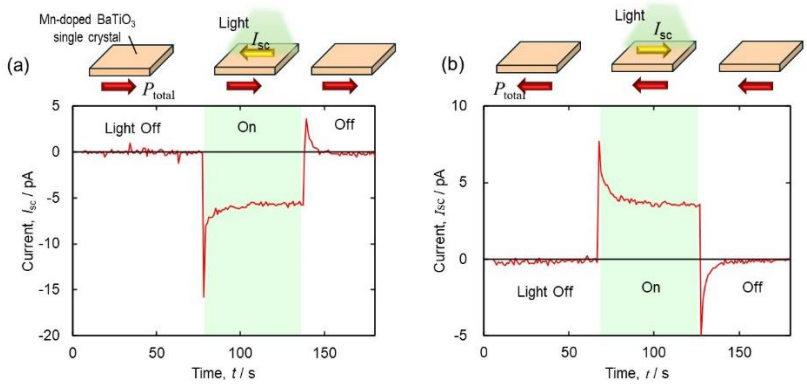



Fig. 2. On/off switching behavior of photocurrents of 1 % Mn-doped $BaTiO_3$ single crystals with (a) positive polarization and (b) negative polarization.

## 3. Research plan for the next year

The lifetime of the excited state induced by the pump pulse at a $h\nu$ that is lower than $E_g$ will be investigated for Mn-doped $BaTiO_3$ single crystals with mixed valence state of $Mn^{2+}$ and $Mn^{3+}$ to further uncover the dynamics of photocarriers and the role of Mn under the visible light irradiation. Moreover, the origin of the light-induced broad absorption peaks observed for the Mn-doped samples will be investigated by combining the TAS measurement and density functional theory (DFT) calculations to clarify the mechanisms of the enhanced PV response by Mn doping.

## 4. List of Papers

Hiroki Matsuo*, Yuji Noguchi
"Impact of Mn doping on the ferroelectric photovoltaic effect in multidomain $BiFeO_3$ thin films under above-bandgap illumination"
***Japanese Journal of Applied Physics*** 62, SM1011 (2023)

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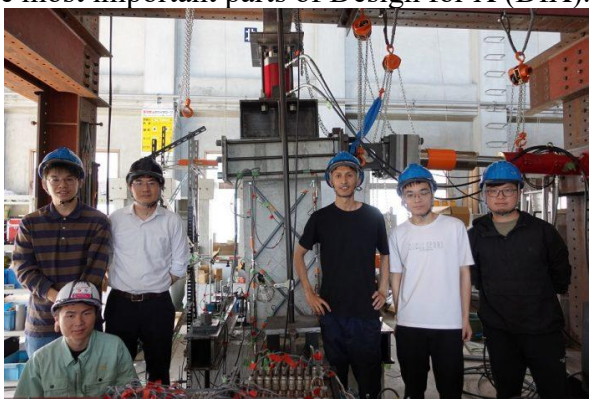
|---|---|---|---|
| No. 2-5-2 | Next-Generation Design of Structures | |  |
| **Cluster Coordinator** | | | |
| Name | Gaochuang CAI | | |
| Affiliation,<br>E-mail | IROAST<br>Email: cai@kumamoto-u.ac.jp | Title | Associate professor |
| Research Field | Environment-friendly technology / Strengthening resilience /<br>Advanced materials / | | |
| **Cluster Members** | | | |
| Name | Affiliation/Title | | |
| Kazuo DAN | Faculty of Advanced Science and Technology, Kumamoto University (KU) / Full professor | | |
| Amir SI LARBI | University of Lyon, France / Full professor,<br>*IROAST Visiting Professor* | | |
| Konstantinos Daniel TSAVDARIDIS | City, University of London, U.K. / Full professor,<br>*IROAST Visiting Professor* | | |
| Danièle WALDMANN | Insitut für Massivbau (Institute of Concrete and Masonry Structures), Technischen Universität Darmstadt, Germany / Full professor | | |

**[Details of activities]**

## 1. Research outline and its perspective

The research unit aims to the two key research themes, i.e., (1) safety and optimization of structures under extreme loads (e.g., strong earthquake, earthquake-fire, etc.) including the application of high-performance materials (See Figure 1 a), and (2) recycling of wastes arising from the extreme loads, in particular the application in the concrete industry, and strengthening the well-designed structures with limited damages subjected to the extreme loads (See Figure 1 b). The two themes also can be shortly called *Design for Structural Safety and Sustainability* (DfS$^3$), one of the most important parts of Design for X (DfX).



(a) High-performance RC walls under strong earthquakes

(b) RC columns under strong earthquakes

Figure 1 Research examples on the topic of DfS$^3$at the cluster

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

The following projects have been conducted in FY2023,

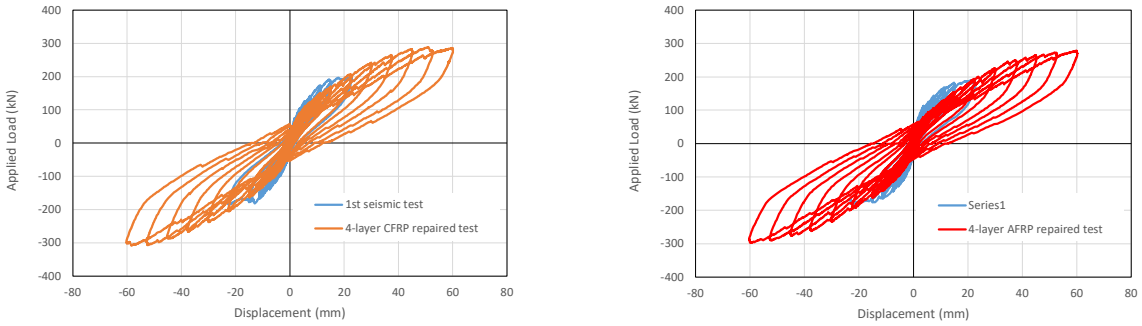
(1) Seismic performance and evaluation method of resilient RC (RRC) walls under multiple reversed cyclic loads induced by strong earthquakes (Test and numerical)
(2) Seismic performance and evaluation method of FRP repaired square RRC columns under multiple reversed cyclic loads induced by strong earthquakes (Test)
(3) Numerical study on seismic performance of reinforced concrete-filled steel tube columns under simulated seismic loads
(4) Numerical study on flexural performance of RC beams with high-strength bars after fire
(5) Experimental and numerical study on shear performance of RC beams with high-strength bars after fire

The results of two representative projects are summarized here,

(1) Experimental study on seismic performance of CFRP-repaired RRC columns under strong earthquakes

The repair test of RRC (resilient reinforcement concrete) columns has been carried out this year. The following is a summary of the learning situation and test results obtained. After the RRC columns in this test experienced the initial damage stage (the displacement angle reached 3%), it was first repaired with high-strength mortar, then internal pressure filling was used to inject epoxy resin according to the location of the crack, and finally, it was wrapped with different layers or types of FRP (fiber reinforced polymer) cloth, five test specimens have been repaired so far, namely the control specimen, 4 layers of CFRP (carbon fiber reinforced polymer) reinforcement, 6 layers of CFRP reinforcement, 4 layers of AFRP (aramid fiber reinforced polymer) reinforcement, and external steel plate 4 layers of CFRP cloth reinforcement. The loading system of the reinforced specimen is consistent with the initial damage stage, using displacement control, with two cycles at each displacement angle. Figures 2 and 3 show the repair and test results of two representative specimens.

Figure 2 Wrapping of CFRP sheet

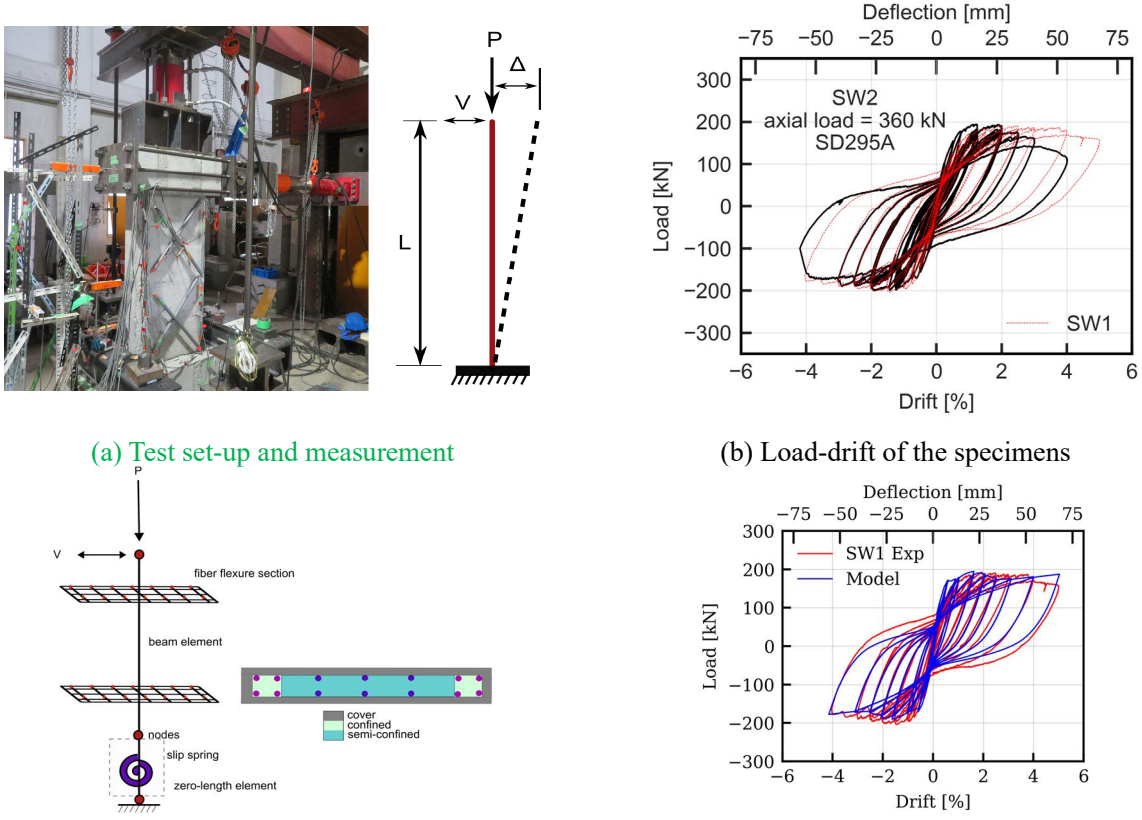



(b) CFRP-repaired specimen (c) AFRP-repaired specimen

Figure 3 Load-displacement of two representative repaired RC specimens

(2) Experimental study on seismic performance of resilient RC walls under strong earthquakes

This study presents an experimental investigation into the seismic behavior of RC shear walls subjected to MRC loading, simulating the effects of LPGM under quasi-static conditions. Two identical specimens, SW1 and SW2, with a span ratio of 2.12, were tested under NC and MRC loading, respectively. The axial load ratio for both specimens was maintained at 0.1 and both specimens failed by shear-flexure failure. Under MRC loading, yield load, maximum load, and failure occurred at lower drift compared to NC loading. The noticeable variation in the load-drift curve is observed after 2% drift. The load-drift curve's envelope exhibits dependency on the load path, with multiple repetitions of loading under MRC, the shear wall experiences greater strength deterioration. The residual drift increases after 0.75% drift in MRC loading compared to NC loading. This observation highlights the vulnerability of the shear wall structure to collapse during LPGM events at lower intensity. The impact of the loading path is less significant on the stiffness of the shear wall. However, the energy dissipation capabilities of the shear wall, measured in terms of cumulative and hysteric damping coefficient, depend significantly on the load path. The progression of failure caused by previous loading cycles is not significant unless the displacement exceeds that of the previous cycle. The shear wall, modeled using forceBeamColumn elements with a strain penetration model, demonstrated the reliability of the model up to the ascending branch in the load-drift curve of about 3% drift. The agreement of the numerical model with experimental results was comprehensive in terms of initial stiffness, strength loading and reloading curves, residual drift, and area under the hysteric curve.




(a) Test set-up and measurement

(b) Load-drift of the specimens

(c) Simulation model

(d) Simulated curve vs. experimental curve

Figure 4 Seismic test of the specimens and simulation

The following journal papers are under review,

[1] **Cai, G.***, Wen, Y.*, Malla, P., Fujinaga, T., Si Larbi, A. (2024). Effect of axial load and shear span on seismic performance of CFT columns reinforced with end-fixed ultra-high strength

rebars, *Bulletin of Earthquake Engineering.*

[2] Su, Q., Qi, W., Liu, Y., **Cai, G.***, Si Larbi A. (2024) Cracking Damage Analysis of Bridge-Railway Station RC Structures Considering Concrete Shrinkage, Creep, and Environmental Temperature. *Engineering, Construction and Architectural Management.*

[3] Sun, B., Huang, Y., Noguchi, T., **Cai, G.**, Zhao W. (2024) Towards an Improved Concrete Construction Process: A Comprehensive Review of Monitoring Methods and Applications. *Journal of Building Engineering.*

[4] Khan, J.*, Si Larbi, A., Algourdin, N., Mesticou, Z., Aggelis, G., **Cai, G.** (2024). A holistic study on the mechanical behavior and acoustic emissions of textile reinforced mortar (TRM) strengthened reinforced concrete beams in flexure. *Construction and Building Materials.*

[5] Khan, J.*, Si Larbi, A., Algourdin, N., Mesticou, Z., Aggelis, G., **Cai, G.** (2024). Monitoring of acoustic emissions (AE) in TRM composites, and the use of supervised learning for bifurcation of cracking & non-cracking major damage based on AE-features. *Construction and Building Materials.*

[6] Deng, X., Zhao, J.*, **Cai, G.***, Si Larbi, A. (2024) Shear behavior of reinforced concrete beams with high-strength reinforcements after high temperatures. *Construction and Building Materials.*

[7] Khan, J.*, Algourdin, N., Mesticou, Z., **Cai, G.**, Si Larbi, A. (2024). The influence of high temperature exposure on the tensile and cracking behavior of crimped-textile reinforced mortar composites (TRMs). *Construction and Building Materials.*

[8] Tsavdaridis, K.D. McKinley, B., Kacaroglu, B.N., Corfar, D.A. and Lawson, R.M. (2024) Bending Test of Long-Span Ultra-Shallow Floor Beam with Two Lightweight Concretes. *Structures*.

## 3. Research plan for the next fiscal year

According to the current process and results, the following research projects will be conducted next year. These projects will be conducted by two post-doctoral researchers, four Ph.D. students, two master students, and 4 research students at Kumamoto University. Based on the projects, more than 6 journal articles will be published or submitted to international journals.

(1) Numerical analysis of resilient RC (RRC) shear walls under strong earthquakes
(2) Experimental study on seismic performance of square RRC columns under strong earthquakes
(3) Experimental study on seismic performance of CFRP-confined RRC columns under strong earthquakes
(4) Numerical study on seismic performance of CFRP-repaired square RRC columns under strong earthquakes

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

(* means the corresponding author of the papers)

[1] Sun, Y. P., & Cai, G. C*. (2023). Seismic Behavior of Circular Concrete Columns Reinforced by Low Bond Ultrahigh Strength Rebars. *Journal of Structural Engineering*, *149*(9), 04023126. 2023.7. (IF:4.1)

[2] Fuchao Zhao*, Feng Xiong, Gaochuang Cai**, Qi Ge, A. Si Larbi Seismic behavior and simplified hysteretic model of precast concrete wall panels with bolted connections under cyclic loading Engineering Structures, 292, 1, 116562 https://doi.org/10.1016/j.engstruct.2023.116562
**Internship student (2022.01.20-2022.02.25 [online]) in IROAST Research Internship Program **Host professor at Kumamoto University*

[3] Zhu, H., He, Y., Cai, G.*, Cheng, S., Zhang, Y., & Larbi, A. S. (2023). Bond performance of carbon fiber reinforced polymer rebars in ultra-high-performance concrete. *Construction and Building Materials*, *387*, 131646.2023.7 (IF:7.3)

[4] Cai, G.*, Fujinaga, T., Si Larbi, A., Wen, Y., & Malla, P. B. (2023). Cyclic behavior of RCFT columns with large D/t ratio steel tubes: Effect of reinforcement arrangement. *Bulletin of Earthquake Engineering*, *21*(9), 4565-4588.2023.7 (IF:4.6)

[5] Wang, Y., & Cai, G.* (2023). Seismic behavior of square concrete columns confined by FRP-steel composite tube. *Journal of Building Engineering*, *65*, 105754. (IF:6.4)

[6] Zhao, J., Jiang, Y., Cai, G.*, Deng, X., Si Larbi, A. (2024). Flexural stiffness of RC beams with high-strength steel bars after exposure to elevated temperatures. https://doi.org/10.1002/suco.202300934 (IF:3.2)

[7] Reena, C.G., Ananthi, B.G. and Tsavdaridis, K.D. (2023) Column Link Behavior in Eccentrically Braced Composite 3-Dimensional Frames. Buildings. 13(12), 2970

[8] Junaid, K.*, Zyed, M., Nonna, A., Cai, G, Si Larbi, A. (2024). Tensile and cracking behaviour of crimped textile reinforced mortar (TRM) based on digital image correlation. *Construction and Building Materials*, 417, 135321.

**5. List of awards, grants, and patents**

-Grants

Seismic Performance and AI-based Evaluation Method of SRC Rectangular Columns Subjected to Multiple Repeated Cyclic Loads

Research Grant Ohata Foundation, 2,000,000JPY, 2022.10-2023.9

JST Sakura Science Exchange Program, Advanced technology and risk analysis of structures under extreme loads or environments（極端な負荷または環境下にある構造物の高度なテクノロジーとリスク分析）, 3,323,395JPY, 2024.1.22-2024.1.28

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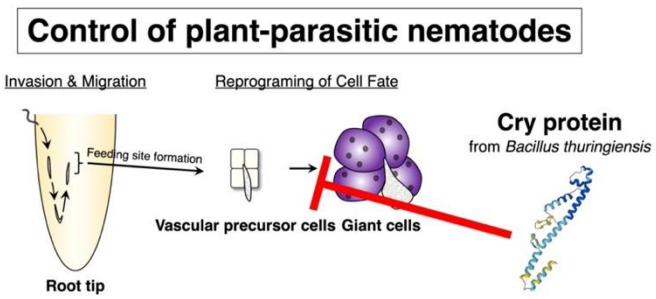
|---|---|---|---|
| No. 2-5-3 | Control of Plant-parasitic Nematodes | |  |
| **Cluster Coordinator** | | | |
| Name | Masahiko FURUTANI | | |
| Affiliation, E-mail | IROAST | Title | Associate Professor |
| Research Field | Environmental bioscience | | |
| **Cluster Members** | | | |
| Name | Affiliation/Title | | |
| Shinichiro SAWA | Faculty of Advanced Science and Technology, Professor | | |
| Raffi AROIAN | University of Massachusetts Medical School, Professor | | |

**[Details of activities]**

## 1. Research outline and its perspective

*Bacillus thuringiensis* crystal (Cry) proteins are specifically toxic to the insect orders Lepidoptera, Coleoptera, Hymenoptera and Diptera, and also to nematodes. In this Research Cluster "Control of plant-parasitic nematodes", we are going to develop and validate new methods of plant-parasitic nematode control using Cry proteins. Cry proteins will be expressed in the root at a particular time during nematode infection to investigate the effective expression of Cry proteins in plants. In addition, we will visualize the Cry toxicity pathway from plant cells to nematodes by expressing fluorescent fusion protein mCherry−Cry.




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

Previously, Dr. Aroian have shown that when Cry5B and Cry6A were transiently expressed in tomato roots, these proteins reduced slightly plant-parasitic nematode infection. In this project, we are planning to express these Cry proteins stably by creating stable transgenic plants in order to analyze the detailed role of Cry proteins in the control of nematode infection. This year, codon-optimized Cry5B and Cry6A for Arabidopsis were cloned into the inducible system, pER8 a binary vector. At the same time, to analyze the localization of the Cry proteins during nematode infection, Cry5B and Cry6A were fused with the fluorescent protein mCherry. pER8 $G_{10\text{-}90}$p<<mCherry-Cry6A was transformed into Arabidopsis and transgenic lines are under selection.

## 3. Research plan for the next year

Using the transgenic plants pER8 $G_{10\text{-}90}$p<<mCherry-Cry6A, the effects of the Cry6A protein on nematode infection will be analyzed by counting the number of galls in roots where the expression of mCherry-Cry6A is induced. In addition, to check the level of Cry6A expression and the protein

localization during nematode infection, the fluorescence of mCherry-Cry6A will be detected by confocal microscopy. Although the protein structure of Cry6A was revealed, the role of the domain remains unknow. To elucidate the mechanism of action of Cry6A, truncated Cry6A will be expressed during nematode infection.

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

Not applicable.

**5. List of awards, grants, and patents**

Principal Investigator (PI)

1. Kakenhi, Grant-in-Aid for Scientific Research (C) (2023-2025), Liquid-liquid phase separation in polar auxin transport.

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|---|---|---|---|
| No. 2-5-4 | Low-Dimensional Molecular Electronics and Spintronics | | |
| **Cluster Coordinator** | | | |
| Name | Zhongyue ZHANG | | |
| Affiliation,<br>E-mail | IROAST<br>zhongyuezhang@kumamoto-u.ac.jp | Title | Associate Professor |
| Research Field | Advanced materials | | |
| **Cluster Members** | | | |
| Name | Affiliation/Title | | |
| Yufan LI | Assistant Professor, The Chinese University of Hong Kong | | |
| Zhenfei LIU | Assistant Professor, Wayne State University (USA) | | |

**[Details of activities]**

**Research Outline and Perspectives:**
The target of this research cluster is to provide comprehension to the unique physical properties of achieved molecular materials. As a result, the coordinator invited one physicist (Yufan Li) with the expertise of magnetism, superconductivity and spintronics and one theoretical chemist (Zhenfei Liu) with the expertise of theoretical simulations of the molecular electronic structures. We intended to unveil the spin selective transport behavior of single molecules via inverse spin Hall effect and interpret the electron-phonon coupling via theoretical calculations.

**Research Activities:**
**Collaboration with physicist:** The coordinator, Prof. Zhang visited the lab of Prof. Li in Hong Kong by the end of August and discussed about the possible collaboration on the molecular spintronics. Since Prof. Li just started his independent career in Hong Kong and the instruments have not been perfectly set up, they discussed about the potential experiment schemes that could be performed in near future. (**Fig.1**) The discussion was mainly focused on the detection of chirality induced spin filtering effect using inverse spin Hall effect, and the major challenge in this scheme is to find a correct fabrication method that allows the spin current to diffuse through the molecular layer.

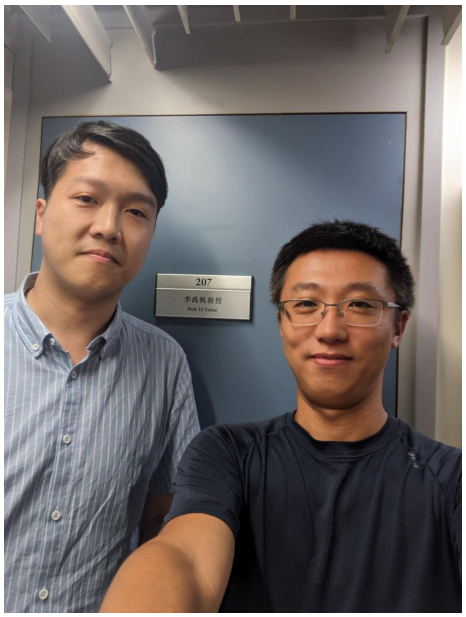


**Fig.1** Discussion with Prof. Li in Chinese University of Hong Kong.

**Collaboration with theoretical chemist:** Prof. Zhang has already been collaborating with Prof. Liu since 2022 and examined the evolution of electronic structure in the solid-state electrochemical process of 2D-MOF, CuTHQ. In the fiscal year of 2023, two

works have been collaborated with Prof. Liu. The first one was the calculation of charge transfer at the interface of heterojunction composed by multiple 2D MOFs (CuTHQ and $Ni_3BHT_2$). The calculation results clearly suggested the HOMO and LUMO orbitals located in different MOFs, which is a firm indicator of charge transfer. Unfortunately, the $Ni_3BHT_2$ MOF cannot be prepared as a crystalline material, which significantly enhanced the difficulty of fabricating MOF heterojunctions. The second project was the calculation of the electronic structures of recently achieved 2D MOFs: $Cu_3(Trip\text{-}H)_2$ and $Cu_3(Trip\text{-}Me)_2$. The band structure calculation suggested these two MOFs are both semiconductors with a large band gap about nearly 2.5eV. Interestingly, a nearly flat band was observed at Fermi level. These band structures suggested some potential unusual electronic properties, such as large effective mass and magnetic field responsive transportation of electrons in these MOFs. Further work will be focused on the correlation between the physical properties and the band structure calculations between these MOFs. (**Fig.2**)

**Research plan for the next fiscal year:**

Two works are going to be attempted in the next fiscal year. Firstly, we will finalize the upper mentioned work of new 2D MOFs, understand their electronic properties and try to publish these results. On the other hand, we would like to accelerate the study of using helical single molecules as the spin filter, and to understand the mechanism of the spin selectivity of these molecules via the characterization of electron-phonon interaction.

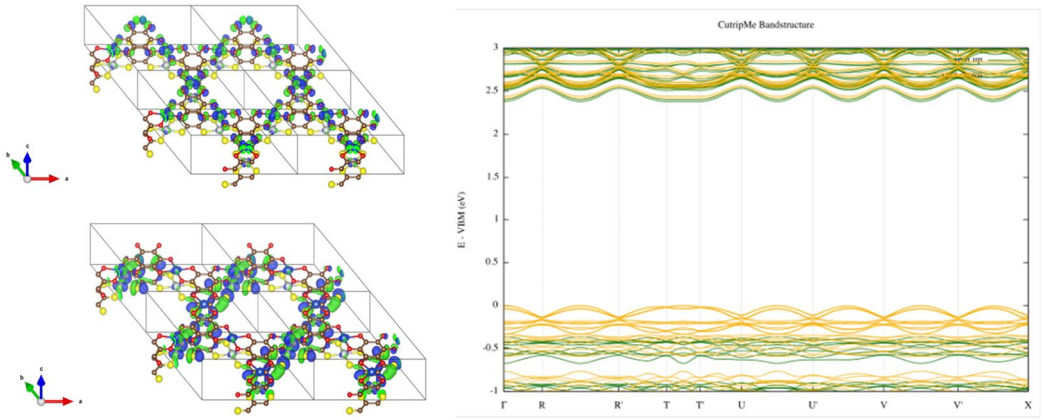


**Fig.2** Left, HOMO-LUMO diagram of CuTHQ-NiBHT heterostructure. Right, band structure of $Cu_3(Trip\text{-}Me)_2$

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|---|---|---|---|
| No. 2-5-5 | Development of Nano and Supramolecular Materials | |  |
| **Cluster Coordinator** | | | |
| Name | Shinya HAYAMI | | |
| Affiliation,<br>E-mail | Faculty of Advanced Science and Technology<br>hayami@kumamoto-u.ac.jp | Title | Professor |
| Research Field | Environmental bioscience / Environment-friendly technology / Advanced materials | | |

| **Cluster Members** | |
|---|---|
| Name | Affiliation/Title |
| Shintaro IDA | Kumamoto University / Professor |
| Yoshihiro SEKINE | Kumamoto University / Associate Professor |
| Zhongyue ZHANG | Kumamoto University / Associate Professor |
| Michio KOINUMA | Kumamoto University / Associate Professor |
| Jorge BELTRAMINI | Queensland University of Technology / Professor, *IROAST Visiting Professor* |
| Yang KIM | Kosin University / Professor |
| Martino DI SERIO | University of Naples Federico II / Professor, *IROAST Visiting Professor* |
| Shie-Ming PENG | National Taiwan University, *IROAST Visiting Professor* |
| Parasuraman SELVAM | Indian Institute of Technology-Madras, *IROAST Visiting Professor* |

**[Details of activities]**

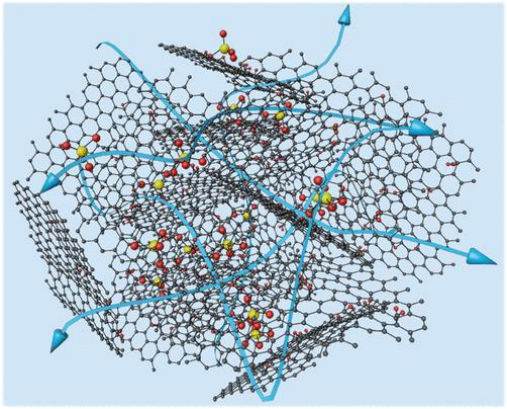
## 1. Research outline and its perspective

Graphene oxide (GO) has been considered as only a precursor for graphene but also one of the most promising materials because of its excellent properties such as photoluminescence, ferromagnetism, electrodes, and water permeation. As it is now, it is said that GO has wider range of applications than graphene. Therefore, it is important for industrial development to study GO. Recently, we focused on (i) ion conduction for fuel cell, (ii) biomass conversion reaction, (iii) agri-bio application by using GO nanosheet and its derivatives.

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

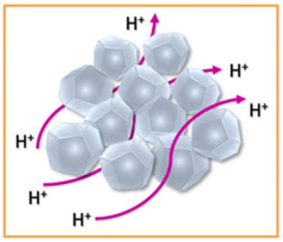
### (i) Three-Dimensional Sulfonated Graphene Oxide Proton Exchange Membranes for Fuel Cells

During the last decades, graphene oxide (GO)-based materials have been extensively studied as low-cost efficient solid electrolytes for fuel-cell application. However, the observed limited proton conductivity of GO in the out-of-plane directions and associated lower fuel-cell performance largely limit their practical application. Herein, we have demonstrated a sulfate ion-intercalated three-dimensional graphene oxide (3DSGO) showing an exceptionally high out-of-plane proton conductivity of 0.74 S cm–1 at room temperature and 90% RH, and an in-plane proton conductivity of 3.19 S cm–1. Additionally, measurement of cell performance using the prepared membrane as the electrolyte of the proton exchange membrane fuel cell (PEMFC) showed an optimum power density of 112.65 mW cm–2 at 100% RH and 30 °C, which is more than double that achieved for 3DGO (50 mW cm–2). This efficient proton conduction ability and PEMFC performance of the 3DSGO is linked with the 3D interconnected ionic highways and substantial interlayer void space, which provide the higher water retention capacity in the 3D spongy architecture and a facile proton conduction pathway.



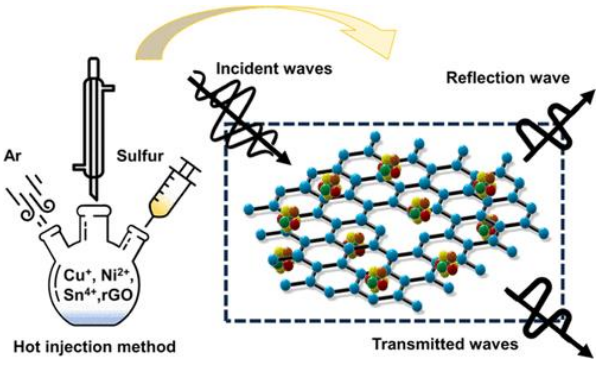
**(ii) Thermally stable proton conductivity from nanodiamond oxide**

we report nanodiamond oxide (NDOx), obtained from modified Hummers' oxidation of nanodiamond (ND), showing excellent proton conductivity and thermal stability. NDOx possesses hydrophilicity resulting in higher water adsorption and the retention of functional groups at elevated temperatures can be attributed to the high proton conductivity and thermal stability, respectively.




**(iii) development of advanced electromagnetic wave absorbing materials**

The development of advanced electromagnetic wave absorbing materials capable of simultaneous dual/multiple frequency bands has received widespread attention due to their potential to mitigate electromagnetic interference and enhance communication technologies. Herein, we report efficient dual frequency band electromagnetic wave (EMW) absorption from a hybrid of high-purity Cu2NiSnS4 (CNTS) nanoparticles and reduced graphene oxide (rGO) (CNTS/rGO). The surface morphology and physicochemical properties of prepared materials (pure CNTS and CNTS/rGO with different rGO filling ratios) were characterized using powder X-ray diffraction (PXRD), Raman spectroscopy, transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), and scanning TEM (STEM) analysis. The electromagnetic-wave-absorption performances were conducted using a vector network analyzer with the frequency ranging between 2 and 18 GHz. The complex permittivity, magnetic permeability, dielectric loss tangent, magnetic loss tangent, dielectric relaxation phenomena (Cole–Cole plot), eddy current loss parameter, and attenuation constant values related to the electromagnetic wave absorption of the materials have been studied. The experimental results confirmed that CNTS and CNTS/rGO composite materials can absorb different electromagnetic wave frequency bands. Significantly, CNTS/rGO (50%) exhibits exceptional electromagnetic-wave-absorption properties across dual frequency bands with the optimal absorption loss of −38.2 dB at 17.1 GHz and a broad absorption peak of −10.4 dB at 5.6 GHz, offering significant potential for use in various technological applications, including



stealth technology, wireless communication, and radar systems. The enhanced microwave-absorption properties of the material can be attributed to the successful design of a well-dispersed heterostructure of CNTS/rGO containing different phases, including a hybrid of dielectric and magnetic material along with the efficient dielectric loss, magnetic loss, and their synergistic contribution in the electromagnetic wave absorption. The outcomes of this research can lead to technological advancements, improved functionality, and future direction to pressing challenges in today's interconnected world.

## 3. Research plan for the next fiscal year

The future growth of carbon-based materials towards the goal of large-scale commercialization of the technologies largely depends on the better understanding and the subsequent control on the carbon substrate. The fabrication of ideal nano-architecture with appropriate surface texture (size, shape, porosity) and low cost are the primary concern to achieve the maximum performance from the energy conversion and storage device. In the case of electrode support materials for PEMFCs and SCs electrodes, the suitable structures and morphologies of the materials can promote the exposure of active sites to increase the catalytic activity/charge storage and enhance long-term stability. The possible new directions to prepare advanced nano-structure from carbon allotropes include the fabrication of a unique 3D network with interconnected pores from the blending of 0D CQDs, 1D CNTs and 2D graphene sheets. The well-fitted compositions with a homogeneous mix-up of components allow unique synergistic effects, in which each unit exerts its own advantages and overcomes the deficiencies of the other units. In addition, the introduction of heteroatoms is capable of increasing the active sites, molecular structure, bandgap and charge mobility. Thus, the materials have a strong influence on the performance.

On the other hand, graphene oxide (GO), one of the nanomaterials, is a nanosheet material with many oxygen functional groups. Its high water content and ability to supply water and adsorb salts prevents salt damage and makes it possible to promote plant growth and forest improvement using GO soil. The large number of oxygen functional groups enables effective decomposition and conversion of biomass through strong interactions such as hydrogen bonding and oxidizing power. We will conduct mass synthesis of graphene oxide (GO) nanosheet materials suitable for each application, and promote demonstration experiments for CO2 reduction and biomass supply, such as promotion of plant growth in barren areas and forest improvement in GO soils, and develop highly efficient, highly selective, and innovative biosynthesis of GO and GO hybrids from agricultural and wood wastes and other biomass. The project targets the development of biofuels through innovative biomass decomposition and conversion reactions with high efficiency and high selectivity, using GO as a base and catalyst material, and developing biofuels with high efficiency and high yield based on the promotion of plant growth and forest improvement in GO soil and the decomposition and conversion of biomass with GO in a water-soluble, one-pot reaction. Development of biofuels with high efficiency and high yield based on the decomposition and conversion of biomass by water-soluble and one-pot reactions with GO. Furthermore, by mixing GO with seawater, we aim to establish a social infrastructure for recycling systems based on the SDGs, such as CO2 reduction, by realizing desalination from seawater for agricultural use with a simple method.

## 4. List of journal papers


1. Z. Cai, M. S. Islam, M. Fukuzaki, M. A. Rahman, J. Matsuda, Z. Zhang, Y. Sekine, B. Bateer, S. Hayami, $Cu_2NiSnS_4$ Nanoparticles Supported on rGO for Dual Frequency Range Electromagnetic Shielding, ACS Appl. Nano Mater., 6, 23, 21980–21990 (2023). DOI: 10.1021/acsanm.3c04196
2. L. I. Ardhayanti, Md. S. Islam, M. Fukuda, X. Liu, Z. Zhang, Y. Sekine, S. Hayami, Thermally stable proton conductivity from nanodiamond oxide, Chem. Commun., 59, 8306-8309 (2023). DOI: 10.1039/D3CC02016A

## 5. List of awards, grants, and patents

KAKENHI, Grant-in-Aid for Challenging Research (Exploratory) 2022-2023

<table>
<tr><td>No. 2-5-6</td><td colspan="3">Plant Cell and Developmental Biology</td><td rowspan="3">  </td></tr>
<tr><td colspan="4">Cluster Coordinator</td></tr>
<tr><td>Name</td><td colspan="3">Sinichiro SAWA</td></tr>
<tr><td>Affiliation,<br>E-mail</td><td>Faculty of Advanced Science and Technology<br>（FAST）/ International Research<br>Center for Agricultural and Environmental Biology<br>（IRCAEB）<br>Email: sawa@kumamoto-u.ac.jp</td><td>Title</td><td colspan="2">Professor</td></tr>
<tr><td>Research Field</td><td colspan="4">Environmental bioscience</td></tr>
<tr><td colspan="5">Cluster Members</td></tr>
<tr><td>Name</td><td colspan="4">Affiliation/Title</td></tr>
<tr><td>Carolina ESCOBAR</td><td colspan="4">University of Castilla La Mancha, Spain / Professor, IROAST Visiting Professor</td></tr>
<tr><td>Bruno FAVERY</td><td colspan="4">CNRS Institut Sophia Agrobiotech, France / INRAE senior scientist (DR2), IROAST Visiting Professor</td></tr>
<tr><td>Mitsuhiro AIDA</td><td colspan="4">FAST / Professor</td></tr>
<tr><td>Takumi HIGAKI</td><td colspan="4">FAST / Professor</td></tr>
<tr><td>Yuki YOSHIDA</td><td colspan="4">FAST / Project Assistant Professor</td></tr>
<tr><td>Hidehiko SUNOHARA</td><td colspan="4">FAST / Visiting Assistant Professor</td></tr>
<tr><td>Reira SUZUKI</td><td colspan="4">FAST / Visiting Assistant Professor</td></tr>
</table>

**[Details of activities]**

## 1. Research outline and its perspective

In this Research Unit, Plant Cell and Developmental Biology, we characterize the molecular and physical mechanisms that contribute to plant development and plant–parasitic nematodes interactions using genetic, biochemical, physiological approaches.

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

Meloidogyne incognita is one of the most detrimental root-knot nematode pests in the world, infecting almost all plant species. The super-growing root culture consists of excised roots from the legume species *Lotus corniculatus* was found to strongly attract infective RKN juveniles, and actively secrete chemo-attractants into the culture media. The chemo-attractant in the culture media supernatant was purified using hydrophobicity and anion exchange chromatography, and was found to be enriched in carbohydrates. Monosaccharide analyses suggest the chemo-attractant contains a wide array of sugars, but is enriched in arabinose, galactose and galacturonic acid. This purified chemo-attractant was shown to contain pectin, possibly rhamnogalacturonan-I, but not

arabinogalactan proteins. More importantly, rhamnogalacturonan-I sidechain groups were found to be essential for RKN-attracting activities. This chemo-attractant appears to be specific to *M. incognita*, as it wasn't effective in attracting other *Meloidogyne* species nor *Caenorhabditis elegans*. Our findings re-enforces pectic carbohydrates as important chemicals mediating micro-organism chemotaxis in the soil, and also highlights the unexpected utilities of the super-growing roots culture system in root pathogen research.

In May 2023, three people visited Bruno Favery's laboratory in France from Kumamoto University to conduct joint research (left photo), hold a joint research meeting (right photo), and discuss the publication of our paper (Oota et al., 2023).

## 3. Research plan for the next year

We will continue collaboration about plant development and biotic interaction.

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

Katogi, T., Yoshida, Y., Nakayama, K., Hoshi, Y., and Sawa, S. (2024) Genome size determination and chromosome characterization of Limosella aquatica L. (Scrophulariaceae) in Japan. Cytologia, 88. 339-346.

Nakagami, S., Notaguchi, M., Kondo, T., Okamoto, S., Ida, T., Sato, Y., Higashiyama, T., Tsai, A, Y-L., Ishida, T., and Sawa, S. (2023) Root-knot nematode modulates plant CLE3-CLV1 signaling as a long-distance signal for successful infection. Science Adv. 9. sciadv.adf4803

## 5. List of awards, grants, and patents

*Principal Investigator*

1. Kakenhi, Grant-in-Aid for Young Scientists (A)
2. JSPS, Fostering Joint International Research (B)

| | | | |
|---|---|---|---|
| No. 2-5-7 | Nano-Organics and Nano-Hybrids | | |
| **Cluster Coordinator** | | | |
| Name | Makoto TAKAFUJI | | |
| Affiliation,<br>E-mail | Faculty of Advanced Science and Technology<br>Email: takafuji@kumamoto-u.ac.jp | Title | Professor |
| Research Field | Advanced materials | | |

**Cluster Members**

| Name | Affiliation/Title |
|---|---|
| Yutaka KUWAHARA | - Faculty of Advanced Science and Technology (FAST), Kumamoto University<br>Assistant Professor |
| Hirotaka IHARA | - Faculty of Advanced Science and Technology (FAST), Kumamoto University<br>Professor Emeritus |
| Nanami HANO | - Faculty of Advanced Science and Technology (FAST), Kumamoto University,<br>- Université de Bordeaux, France<br>JSPS Overseas Research Fellow |
| Reiko ODA | - CNRS, Université de Bordeaux, France<br>Research Director<br>*IROAST Visiting Professor* |
| Josep-Lluis BARONA-VILAR | - Instituto de Historia de la Medicina y de la Ciencia López Piñero (IHMC), Universidad de Valencia, Spain<br>Professor<br>- *IROAST Visiting Professor* |
| Zhenghe XU | - College of Engineering, Southern University of Science and Technology, China<br>Dean, Professor<br>- Department of Chemical and Materials Engineering, University of Alberta, Canada<br>Teck Professor<br>- *IROAST Visiting Professor* |
| Etsuko FUJITA | - Chemistry Division, Brookhaven National Laboratory, USA<br>Senior Scientist Emeritus<br>- *IROAST Visiting Professor* |
| Naoya RYU | - Kumamoto Industrial Research Institute, USA<br>Senior Scientist |

**[Details of activities]**

## 1. Research outline and its perspective

Our research cluster named “Nano-Organics and Nano-Hybrids” at the IROAST focuses on functional nano-objects composed of organics, inorganics and hybrids. Nine members including

four visiting professors from France, Spain, United States and China join the research cluster. The international collaborative projects regarding basic and advanced chemistry on nano-organics and nano-hybrids are initiated and carried out by each member, and their targets are widely distributed across highly diverse fields.

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

2-1. Exchanges of members regarding with international collaboration

We could meet and have fruitful discussion for resent results and future research tasks with following collaborators:

*University of Bordeaux (**UB**), France*

The University of Bordeaux (UB), Kumamoto University (KU) and Kyoto University have applied to the International Research Projects (IRP) as a follow-up to a joint research project "Laboratoire international associé (LIA) - 'Chiral nanostructures for photonic applications' (CNPA)" that has been ongoing since 2015, and the joint research project will continue in the future. In 2023, Mr. Keisuke Kadota (1st year-MS student) studied in the research group of Dr. Reiko Oda (Visiting Professor of IROAST) for six months from October 2023 to March 2024 and conducted research on collaborative research projects. In January 2024, Prof. M. Takafuji and Prof. H. Ihara visited UB and had a discussion on the progress of the joint research project with Dr. N. Hano of the Nano-Organic/Nano-Hybrid Research Unit, who has been working in Dr. Oda's group as a JSPS Overseas Research Fellow since March 2022.

*Universitat de València (**UV**), Spain*

Prof. Barona-Vilar were invited to IROAST of KU in Nov. 2023. We organized the IROAST seminar for his lecture titled "Artificial Intelligence in Health Care. Potentials, risks and ethical impact".

Members of the research cluster of "Nano-organics and Nano-hybrids" (Prof. Makoto TAKAFUJI and Dr. Nanami HANO) visited University of Valencia on July, 2023, and discussed on the research topics including nano-hybrid materials with Prof. Josep BARONA and Prof. Eugenio CORONADO. We discussed extending our exchange activities to include mutual visits and exchange activities between students of both universities. We had meeting with the vice president, Carles Padilla Carmona, and agreed to proceed with preparations for the conclusion of a student exchange agreement in the future.

*University of Dhaka (**UD**), Bangladesh*

An international co-authored paper on the collaboration, which started with the visit of Dr. Shahruzzaman Sumon (Follow-up Research Fellowship of the Japan Student Services Organization (JASSO)) from University of Dhaka in 2022, was published in an international journal.

*Lanzhou Institute of Chemical Physics (**LICP**), Chinese Academy of Sciences (CAS), China*

An international co-authored paper on the collaboration, which started with the visit of researchers (Prof. Hongdeng Qiu, and 4 members) from the Lanzhou Institute of Chemical Physics in 2022, was published in an international journal.

2-2. Maintaining international collaboration by remote-meetings and e-mail discussions with

- ✓ University of Geneva (**UG**), *Swiss Confederation (Switzerland),*
- ✓ Vytautas Magnus University (**VMU**), *Lithuania*
- ✓ Brookhaven National Laboratory (**BNL**), *United States of America,*
- ✓ Noakhali Science and Technology University (**NSTU**), *People's Republic of Bangladesh,* and
- ✓ Kyrgyz-Turkish Manas University (**KTMU**), *Kyrgyz Republic*, and

✓ Baku State University (**BSU**), *Republic of Azerbaijan*

2-3. Publishing with international collaborators
Totally six co-authored papers have been published with researchers of **UB** (four articles), **UD** (one article) and **LICP** (one article) in international journals.

2-4. Grant projects regarding with international collaboration

✓ Development of Soft Encapsulation Technology for Supramolecular Chiral Nanospaces Expressing Tunable Ultra-Enhanced Circular Polarization.
KAKEN, Fund for the Promotion of Joint International Research (Fostering Joint International Research (B)), JSPS, PI: M. Takafuji, Co-PI: N. Ryu, N. Hano, FY 2023-2026.

✓ Circular polarization functions of chiral nano-structure integrated thermo-setting polymer films.
Bilateral Joint Research Project, JSPS. PI: Prof. M. Takafuji, Partner: Dr. Y. Ferrand and Dr. C. Olivier, who are LIA members of **UB**. FY 2022–2024.

✓ Enantioselective nanobioimaging and biological application by fluorescent nanomaterials with controlled chiral space.
Bilateral Joint Research Project, JSPS. PI: Prof. H. Ihara. Partner: Prof. H. Qiu's group of **LICP**. FY 2022–2024.

✓ Development of monovalent ion selective ion exchange membranes based on polymer/MOF for salinity gradient energy production by Reverse Electrodialysis (RED).
Bilateral Joint Research Project, JSPS and TUBITAK (Turkey). PI: Prof. M. Takafuji. Partner: Dr. E. Guler's group of Atilim University (**AU**), Prof. N. Kabay's group of Ege University (**EU**), Prof. A. Tuncel's group of Hacettepe University (**HU**) and Prof. M. Tominaga's group of Sage University (**SU**). FY 2022–2024.

## 3. Research plan for the next year

- We plan to apply to the International Project on Chiral Substances in collaboration with the University of Bordeaux, Tohoku University, and Kyoto University. In addition, the University of Bordeaux side plans to apply for the third phase of the International Research Projects (IRP).
- We will prepare for the conclusion of a student exchange agreement with the University of Valencia.
- We will accelerate our efforts for new international collaborations.

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

4-1. Chiral H-aggregation-induced large stokes shift with CPL generation assisted by $\alpha$-helical poly(L-lysine) substructure
K. Yoshida, Y. Kuwahara, N. Hano, Y. Horie, M. Takafuji, N. Ryu, S. Nagaoka, R. Oda, H. Ihara
***Chirality***, Vol. 35 (7), pp. 411-417, 2023. DOI: 10.1002/chir.23553

4-2. Controlled packing of chiral assembly scaffolds to promote chiral J-aggregation of carbocyanine dyes
N. Ryu, Y. Yamamoto, Y. Okazaki, N. Hano, Y. Iwamoto, T. Shirosaki, S. Nagaoka, R. Oda, H. Ihara, M. Takafuji

***Chemical Communications***, Vol. 59, 11979-11982, 2023. DOI: 10.1039/D3CC03394E

4-3. Sequential chiral induction between organic and inorganic supramolecular helical assemblies for the in situ formation of chiral carbon dots
P. Pranee, A. Scalabre, C. Labrugere, N. Ryu, A. Yano, N. Hano, D. Talaga, Y. Okazaki, E. Pouget, S. Nlate, S. Bonhommeau, M. Takafuji, T. Wada, H. Ihara, T. Buffeteau, D. M Bassani, R. Oda
***Chemical Communications***, Vol. 59, pp.9762-9765, 2023. DOI: 10.1039/D3CC02057F

## 5. List of grants and patents

Accepted grants (On-going project)

5-F1. FY 2023–2026: KAKEN, Fund for the Promotion of Joint International Research (International Collaborative Research)), JSPS, PI: **M. Takafuji**, Co-PI: **N. Ryu**, **N. Hano**, 16,100,000 yen.

5-F2. FY 2021–2024: KAKEN, Grant-in-Aid for Scientific Research (B), JSPS, PI: **M. Takafuji**, Co-PI: **N. Hano**, 13,200,000 yen.

5-F3. FY 2022–2024: KAKEN, Grant-in-Aid for Scientific Research (C), JSPS, PI: T. Shirosaki, Co-PI: **M. Takafuji**, N. Ryu, 3,200,000 yen.

5-F4. FY 2022–2024: KAKEN, Grant-in-Aid for Early-Career Scientists, JSPS, PI: **N. Hano**, 3,500,000 yen

5-F5. FY 2022–2024: Bilateral Joint Research Projects with Turkey, JSPS, PI: **M. Takafuji**, 5,000,000 yen

5-F6. FY 2022–2025: Bilateral Joint Research Projects with China, JSPS, PI: **H. Ihara**, 4,500,000 yen

5-F7. FY 2022–2024: Bilateral Joint Research Projects with France (Open Partnership), JSPS, PI: **M. Takafuji**, 4,000,000 yen

5-F8. FY 2020–2023: KAKEN, Grant-in-Aid for Challenging Research (Exploratory), JSPS, PI: **H. Ihara**, Co-PI: S. Nagaoka, **Y. Kuwahara**, 5,000,000 yen

| | | | |
|---|---|---|---|
| No. 2-5-8 | Nano-medicine and Drug Delivery System | |  |
| **Cluster Coordinator** | | | |
| Name | Hamid HOSANO | | |
| Affiliation,<br>E-mail | Institute of Industrial Nanomaterials（IINa）<br>Email: hamid@kumamoto-u.ac.jp | Title | Professor |
| Research Field | Biotechnology & healthcare technology /<br>Environment-friendly technology | | |

| **Cluster Members** | |
|---|---|
| Name | Affiliation/Title |
| Nushin HOSANO | Institute of Industrial Nanomaterials, Kumamoto University<br>Visiting Associate Professor |
| Konstantinos KONTIS | School of Engineering, University of Glasgow, UK<br>Professor/ Dean for Global Engagement East-Asia & China |
| Firus ZARE | Queensland University of Technology, Australia<br>Professor/ Head of School Electrical Engineering and Robotics |
| Viren Ivor MENEZES | Department of Aerospace Engineering, Indian Institute of Technology Bombay, India<br>Professor |
| Hamid GHANDEHARI | Department of Molecular Pharmaceutics, University of Utah, USA<br>Professor / Chair of Department /Director of Utah Center for Nanomedicine |
| Amir A. FARAJIAN | Department of Mechanical and Materials Engineering, Wright State University, USA<br>Professor |
| Pouyan BOUKANY | Department of Chemical Engineering, Faculty of Applied Sciences, Delft University of Technology, Netherlands<br>Associate Professor |
| Stelios RIGOPOULOS | Department of Mechanical Engineering, Imperial College London, UK<br>Reader |

**Details of activities**

We have been studying the use of physical delivery of drug or reprogramming factors into the cells and tissue, as a safe and reliable method. Our needle-free pain-free disposable vaccine/drug delivery microjet injection has been steadily progressing; new models have been designed and constructed. We have also been exploring integrated diagnostic and therapeutic (theranostics) modalities/nanoparticles/agents, as a unique approach in nanomedicine. The research has potential to be used in a wide range of medical applications.

Our physical delivery approaches are based on applying electrical/mechanical stresses to the cells. In this respect, attention has been made to understand biophysical reactions to reversibly

manipulate the cells by the external stress. We have been investigating promising physical delivery methods including: needle-free painless microinjection, electroporation with nanosecond pulsed electric fields, micro/nano-particle carrier laser-biolistic delivery, sonoporation with microfluidics, and shock waves; which are shown to be appropriate for clinical applications. Particularly we had progress in pain-free non-invasive drug delivery and diagnostic.

With easing travel restrictions (brought by the COVID-19 pandemic) we were hoping to have presence of our Visiting Professors in Kumamoto University; however, this was postponed to the next fiscal year. Meanwhile, with support of IROAST, Hosano could visit Prof. Stelios Rigopoulos at Imperial College London during August 2023 for joint research and publication.
The Cluster soon will welcome new members with diverse research backgrounds. Their presence will promote our projects and will help the Cluster to further achieve its goals.
We will continue our fruitful discussions and collaboration with the cluster members for a joint projects and budget applications.
Our new generation of therapeutic nanoparticles work with Prof. Moosavi-Nejad and Prof. Rigopoulos will continue for the next fiscal year. We also started closer collaboration with them for protein nanoparticles.

Grants:

Grants-in-Aid for Scientific Research, Kakenhi (B), 2021-2025

Joint International publications:

Ziqu Cao, Konstantinos Kontis, Hamid Hosano, Craig White, Ting-Tsung Chang, Muhammed Burak Agir
Vortex Ring Formation Following Shock Wave Diffraction in Low-Pressure Environments
Flow,
Turbulence and Combustion, 111(4) 1127-1138, 2023
DOI: https://doi.org/10.1007/s10494-023-00486-3

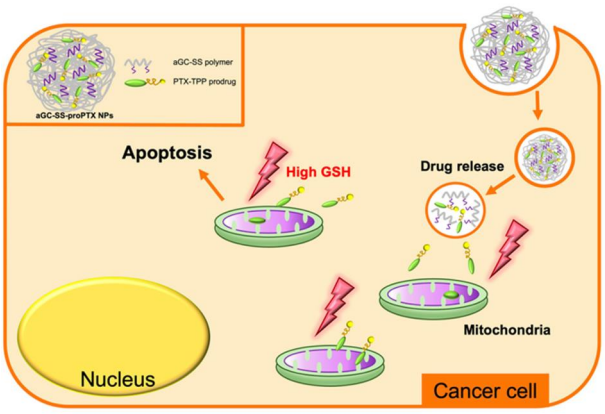
| | | | |
|---|---|---|---|
| No. 2-5-9 | Nano-medicine and Theranostics | |  |
| **Cluster Coordinator** | | | |
| Name | Takuro NIIDOME | | |
| Affiliation, E-mail | Faculty of Advanced Science and Technology<br>Email: niidome@kumamoto-u.ac.jp | Title | Professor |
| Research Field | Biotechnology & healthcare technology | | |

| **Cluster Members** | |
|---|---|
| Name | Affiliation/Title |
| Ick Chan KWON | Biomedical Research Institute, Korea Institute of Science and Technology (KIST), Korea, Principal Research Scientist<br>*IROAST Visiting Professor* |
| Ruda LEE | Institute of Industrial Nanomaterials (IINa)<br>Associate Professor |
| Keiichi MOTOYAMA | Faculty of Life Sciences<br>Professor |
| Taishi HIGASHI | Priority Organization for Innovation and Excellence<br>Associate Professor |

**[Details of activities]**

## 1. Research outline and its perspective

In recent decades, nanocarriers have revolutionized drug delivery with their size advantages and precise targeting capabilities via external stimuli. Nanomedicine has transformed cancer therapies by improving pharmacokinetics, while image-guided drug delivery holds promise for personalized medicine. However, challenges remain, including rapid blood clearance, ineffective nanoparticle transfer in advanced cancer patients, and physiological barriers hindering their efficacy. This research unit is dedicated to developing diagnostic and drug delivery systems for biomedical applications.

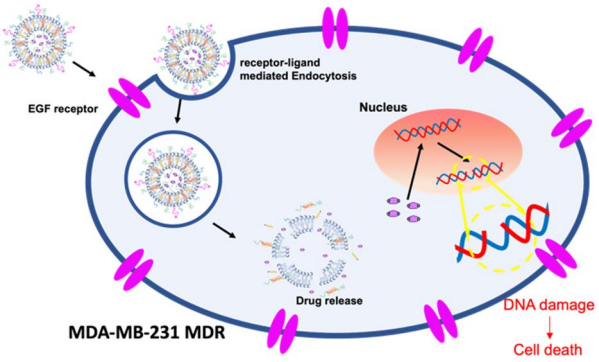



**Schematic illustration of ROS-sensitive Nanomaterials**

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

Nowadays, chemotherapy is still the primary option for cancer therapy. However, the efficacy

of chemotherapy treatment has been severely compromised by the development of multidrug resistance (MDR). Even though much effort has been made to overcome MDR in cancer, limited successes have been achieved with some therapeutic regimens and antineoplastic agents. Recently, amphiphilic block copolymers of Pluronics have been identified to be the most promising MDR reversal agent due to their reversal effect on several distinct drug resistance mechanisms. We modified the target peptide and Pluronics on the carrier and compare the MDR overcoming effect with liposomes. It showed a 10-15 times higher MDR growth inhibition effect on the cellular experiment.




## 3. Research plan for the next fiscal year

Cancer remains a leading global cause of mortality. Chemotherapy has been used for primary conventional treatment for cancer, but multidrug resistance (MDR) poses a significant challenge in chemotherapy. MDR cancer cells often lead to treatment failure due to their ability to develop ways to evade the effects of chemotherapy. It's hypothesized that the dynamic and rapid evolution of tumors in response to treatment will be facilitated by intratumor heterogeneity, contributing to such drug resistance.

Traditional approaches using conventional drugs have encountered limitations in effectively inhibiting MDR cancer cells, addressing the urgent need for novel strategies to combat drug resistance. To overcome drug resistance, a functional nano-drug delivery system has been explored to sensitize the anticancer drugs and minimize their side effects. These systems are applied to overcome MDR via various mechanisms, including bypassing drug efflux and disturbing metabolism. However, the treatment is still a drastic mismatch between effort and return, which calls into question the basic target molecules of MDR cancer cells.

Next year, we will focus on designing and evaluating nanomaterials that overcome multidrug resistance (MDR), advancing toward personalized medicine.

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

1) Ruda Lee, Sho Tanigawa, Yong Il Park, Hoon Kim. Antimetabolite Prodrug Delivery for Non-small Cell Lung Cancer, Korean Society for Biotechnology and Bioengineering Journal, 38: 236-243, 2023

### ** Book publications*

Ruda Lee, Yong Il Park. Exosome detection for early cancer diagnosis. Springer Handbook of Cancer and Immunology, Sep 2023

## 5. List of awards, grants, and patents

Takuro NIIDOME

1) FY2022, Grant-in-Aid for Scientific Research (B)
2) FY2018, JST, CREST

Ruda LEE

1) FY2022 JSPS, Grant-in-Aid for Scientific Research (C)
2) Brain Pool Korea 2022
3) FY2023 Kumamoto Researcher Awards

Ick Chan KWON

1) US patent, Ick Chan Kwon, Ju Hee Ryu, Young-ji Ko, Hye-Sun Kim, Nam-Hyuk Cho, Eun-Jeong Yang, Jae Won Lee. Probe for measuring activity of Caspase-1 and composition for diagnosis of inflammatory diseases containing same. 2023
2) US patent, Ick Chan Kwon, Sun Hwa Kim, YANG Yoosoo, Hyosuk Kim. Method for inducing trans-differentiation of cardiomyocytes based on exosome. 2024
3) US patent, HoWon J Kim, In-San Kim, Jay S Kim, Sun Hwa Kim, Ick Chan Kwon, Jong Won Lee, Yoo Soo Yang, Hong Yeol Yoon. Therapeutic Compounds for Red Blood Cell-Mediated Delivery of an Active Pharmaceutical Ingredient to a Target Cell. 2024

Keiichi MOTOYAMA

1) FY2021 JSPS Grant-in-Aid for Scientific Research (C)

Taishi HIGASHI

1) FY2022 Grant-in-Aid for Scientific Research (B)
2) A-step Ikuseigata
3) The Leading Initiative for Excellent Young Researchers

| | | | |
|---|---|---|---|
| No. 2-5-10 | Quantification of Three Dimensional Vascular Network | |  |
| **Cluster Coordinator** | | | |
| Name | Toshifumi MUKUNOKI | | |
| Affiliation,<br>E-mail | mukunoki@kumamoto-u.ac.jp | Title | Professor |
| Research Field | Biotechnology & healthcare technology / Environmental bioscience / Environment-friendly technology / Strengthening resilience / Advanced materials / Data science and AI | | |
| **Cluster Members** | | | |
| Name | Affiliation/Title | | |
| Yuichiro ARIMA | International Research center for medical sciences, Kumamoto University | | |
| Patrice DELMAS | The University of Auckland, New Zealand, Associate Professor,<br>*IROAST Visiting Professor* | | |

**[Details of activities]**

**1. Research outline and its perspective**

In this project, we aimed to extract vascular information from microspaces and obtain quantitative data based on image information obtained using high-resolution CT. Previous studies have successfully depicted the microvasculature within the heart by adjusting the amount of contrast agent (Figure 1). However, due to the difficulty in evaluating the entire vascular bed, we have also pursued analysis using images obtained with a microscope to perform quantitative assessments (Figure 2).

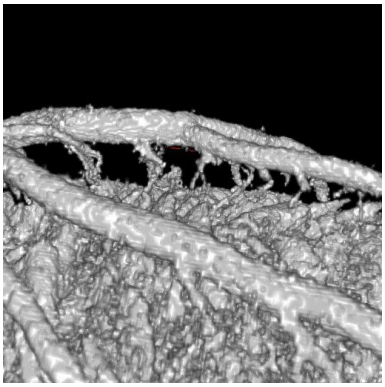


Figure 1: Vessels of the heart imaged with nano CT, enabling evaluation down to 1.5 microns per voxel.

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

In microscope images, it is possible to uniformly stain the entire vascular bed using immunohistochemical staining. With this method, we aimed to acquire vascular information and identify cells that comprise the vasculature and those that do not (in this case, myocardial cells) based on their positional information. In addition to conventional methods using machine learning, we established a method to identify vascular constituent cells with higher accuracy by incorporating cytological characteristics (Table1). Furthermore, we succeeded in creating an algorithm to delineate centerlines from the obtained vascular bed information and comprehensively measure parameters such as branch numbers and branch angles.

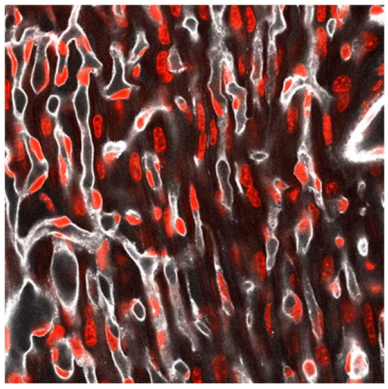


Figure 2: Vessels (white) and cell nuclei (red) stained in microscope images. Although it's a narrow range, it's possible to depict all the vessels.

Table 1: Comparison of algorithms for identifying vascular constituent cells using machine learning (3D CNN), conventional methods, and the new method we developed, confirming high accuracy with our developed approach.

| Method | Precision | Recall | F1-score |
|---|---|---|---|
| 3D CNN | 0.769 | 0.790 | 0.778 |
| Conventional | 0.856 | 0.941 | 0.896 |
| New | 0.860 | 0.946 | 0.901 |

## 3. Research plan for the next fiscal year

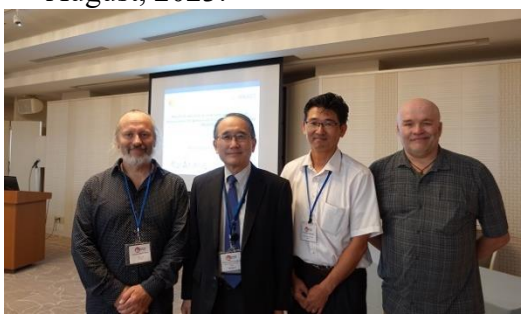
We will apply the classification method established in microscope images to CT images and work on the quantitative evaluation of vascular beds in microspaces. Additionally, we will continue to improve contrast agents to establish a contrast technique capable of depicting the details of microvessels.

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

None

## 5. List of awards, grants, and patents

We organized International Symposium, ACIVIS2023 supported by IROAST at Kumamoto in August, 2023.



With Director Takashima

At the venue (KKR Hotel Kumamoto)

Prof. Mukunoki

Visiting Prof. Delmas

Poster Presentation

| | | | |
|---|---|---|---|
| No. 2-5-11 | Advanced Structural Materials | |  |
| **Cluster Coordinator** | | | |
| Name | Yoji MINE | | |
| Affiliation,<br>E-mail | Faculty of Advanced Science and Technology<br>mine@msre.kumamoto-u.ac.jp | Title | Professor |
| Research Field | Advanced materials | | |

| **Cluster Members** | |
|---|---|
| Name | Affiliation/Title |
| Yufeng ZHENG | School of Materials Science and Engineering, Peking University, China<br>International Research Organization for Advanced Science and Technology (IROAST), Kumamoto University, Japan<br>/ Professor & IROAST Distinguished Professor |
| Paul BOWEN | School of Metallurgy and Materials, University of Birmingham, UK<br>/ Feeney Professor of Metallurgy & *IROAST Visiting Professor* |
| Yu-Lung CHIU | School of Metallurgy and Materials, University of Birmingham, UK<br>/ Professor of Physical Metallurgy |
| Hiroto KITAGUCHI | School of Metallurgy and Materials, University of Birmingham, UK<br>/ Senior Research Fellow |
| Martin DIENWIEBEL | The Institute for Applied Materials - Reliability and Microstructure (IAM-ZM), Karlsruhe Institute for Technology (KIT), Germany<br>/ Professor for Applied Nanotribology & *IROAST Visiting Professor* |
| Robert WILSON | CSIRO, Australia<br>/ Team Leader of Alloys and forming Processes Team |
| Kazuki TAKASHIMA | IROAST, Kumamoto University, Japan<br>/ Distinguished Professor |
| Kwangsik KWAK | Faculty of Advanced Science and Technology, Kumamoto University, Japan<br>/ Assistant Professor |

**[Details of activities]**

## 1. Research outline and its perspective

The mechanical properties of materials are dominated by their microstructures such as grain size, precipitates, phase boundary, grain boundary, etc. In our research group, we aim to clarify the mechanical properties at microscopic level, including tensile properties, fracture and fatigue properties, using the micromechanical testing technology that we have developed (Fig. 1). Furthermore, in conjunction with crystal plasticity finite element simulation, we aim to predict the mechanical properties of bulk materials based on those at microscopic scale. The results obtained

in this research will contribute for developing toughening design of advanced materials.

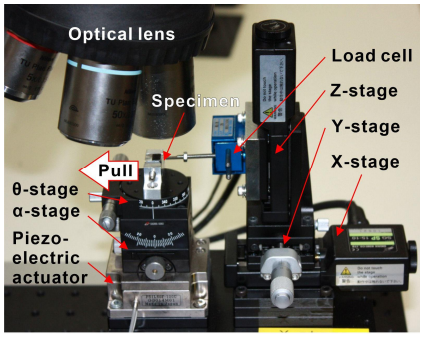


Fig. 1 Micro-mechanical testing machine.

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

Some new and valuable results were obtained in FY2023. The international workshop between **CSIRO** and **KU** was held online in June to exchange information and ideas on the fabrication and mechanical characterization of advanced materials. Dr. **Willson** visited **KU** in November and discuss the sample preparation. In March, Professor **Takashima** visited CSIRO and received additively manufactured titanium alloy samples. We have also collaborated with Professor **Bowen** and researchers (Professor **Chiu** and Dr. **Kitaguchi**) at the **University of Birmingham** (UoB) to elucidate the mechanisms of plastic deformation and fatigue crack propagation in martensitic steel and titanium alloy using the micro-fatigue testing technique developed by KU. Dr. **Kitaguchi** visited **KU** in January and discuss a new collaborative study of nickel super alloys. We have performed metallographic examination on the deformed microstructure of titanium alloy after fatigue in KU and have published an international joint paper entitled “Effects of crystallographic orientation and lamellar configuration on the fatigue crack propagation in a single-colony structure of Ti–6Al–4V alloy” by “S. Ueki, **Y. Mine**, X. Lu, **Y.L. Chiu**, **P. Bowen** (**UoB**) and **K. Takashima**”. Further, Dr. Kwak visited Professor **Dienwiebel** at KIT from August to September to accelerate the collaborative study on the tribology of bearing and austenitic stainless steels.

## 3. Research plan for the next year

Dr. **Kwak** will start a collaborative study with Dr. **Willson** at **CSIRO** about the micro-mechanical characterization of additively manufactured titanium alloys. Professor **Mine** will participate in the 24th European Conference on Fracture in August to deliver an international joint paper entitled “MICROSTRUCTURAL FATIGUE CRACK GROWTH IN SINGLE COLONY OF TI-6AL-4V LAMELLER ALLOY” collaborated with **UoB**. Our graduate student will visit Professor **Dienwiebel** at **KIT** from August to September to accelerate the collaborative study on the tribology/fatigue of bearing steel in hydrogen environment. Professor **Zheng** at **PU** will visit KU in September to wright an international joint paper on the mechanical characterization study of biomaterials.

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

(1) S. Ueki, **Y. Mine**, **Y.L. Chiu**, **P. Bowen**, **K. Takashima**:
Effects of crystallographic orientation and lamellar configuration on fatigue crack propagation in single-colony structures of Ti–6Al–4V alloy: Alternating shear crack growth vs. damage accumulation crack propagation
Mater. Sci. Eng. A, 890 (2024) 145885.

(2) G. Li, D. Chen, **Y. Mine**, **K. Takashima**, **Y. Zheng**:
Fatigue behavior of biodegradable Zn-Li binary alloys in air and simulated body fluid with pure Zn as control
Acta Biomater., 168 (2023) 637–649.

(3) Q. Jia, Q. Jia, S. Zhu, **Y. Zheng**, **Y. Mine**, **K. Takashima**, S. Guan:
A promoting nitric oxide-releasing coating containing copper ion on ZE21B alloy for potential vascular stent application
Journal of Magnesium and Alloys, 11 (12), 4542-4561 (2023) .

## 5. List of awards, grants, and patents

(1) Elucidation of plastic deformation mechanism of additively manufactured Ti-6Al-4V alloys using trans-length scale mechanical characterization, KAKENHI Grant-in-Aid for Early-Career Scientists 2021-2024 (Continuing).

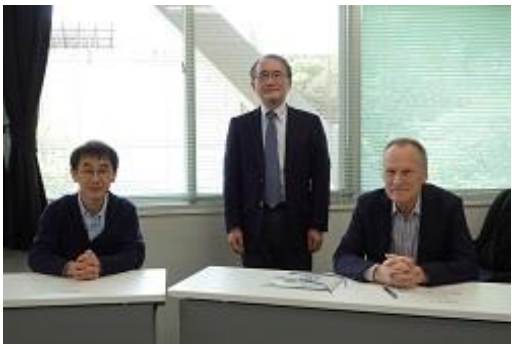
(2) Elucidation of fatigue crack growth mechanism of martensite steels using micro-mechanical testing technique and application to fatigue strengthening design, KAKENHI Grant-in-Aid for Scientific Research (A) 2020-2024 (Continuing).

| | | | |
|---|---|---|---|
| No. 2-5-12 | Microstructure Analysis and Grain Boundary Engineering | |  |
| **Cluster Coordinator** | | | |
| Name | Sadahiro TSUREKAWA | | |
| Affiliation,<br>E-mail | Faculty of Advanced Science & Technology<br>turekawa@kumamoto-u.ac.jp | Title | Professor |
| Research Field | Advanced materials | | |
| **Cluster Members** | | | |
| Name | Affiliation/Title | | |
| Dmitri Aleks MOLODOV | Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany<br>Professor, IROAST Distinguished Professor | | |
| Pavel LEJČEK | Institute of Physics, Czeck Academy of Sciences, Czech Republic<br>Professor, *IROAST Visiting Professor* | | |
| Mitsuhiro MATSUDA | Faculty of Advanced Science and Technology (FAST)<br>Associate Professor | | |
| Thomas WAITZ | Faculty of Physics, University of Vienna, Austria<br>Associate Professor, *IROAST Visiting Professor* | | |
| Christian RENTENBERGER | Faculty of Physics, University of Vienna, Austria<br>Associate Professor, *IROAST Visiting Professor* | | |
| Yoshitaka MATSUKAWA | Faculty of Advanced Science and Technology (FAST)<br>Associate Professor | | |

**[Details of activities]**

S. Tsurekawa's (ST) group:

Professor Tsurekawa has collaborated with Prof. Dmitri A. Molodov (RWTH Aachen University) and Prof. Pavel Lejček (Institute of Physics, Czech Academy of Sciences), who are Distinguished Professor and Vising Professor of IROAST, respectively, in the research field of grain boundary engineering for many years. On the occasion of Prof. D. A. Molodov's (DM) visit to Kumamoto University in May 2023, DM gave two lectures on "Grain Boundary Migration" as part of Prof. Tsurekawa's regular course on Materials Interface Science for GSST. In addition, DM and ST discussed the results of their collaborative work on grain boundary-dislocation interaction using Al bicrystals. DM also stayed at KU in October 2023 and discussed with students of Tsurekawa group about their individual research and provided useful comments.




(At the meeting with Director of IROAST in May 2023)


(Lectures on "Grain Boundary Migration" at the 94th and 95th IROAST Seminars)


Prof. P. Lejček stayed at Kumamoto University in Feb. 2024 and gave a special lecture on "Introduction to grain boundary segregation", focusing on experimental and theoretical methods of studying solute segregation at grain boundaries. In September, PL hosted a master student at his institute and supervised her experimental work on the microstructure evolution of a high entropy alloy. In addition, PL provided a special online lecture at a meeting of the Iron and Steel Institute of Japan (ISIJ) research project, "*Approach of grain boundary engineering for achieving high-permance steels*" on March 18, 2024 in Tokyo.


(Lecture on "Introduction to grain boundary segregation" at the 117th IROAST Seminar)

M. Matsuda's (MM) group:

Many of functional materials, such as semiconductor, super conductor, solar cell, magnetic materials and shape memory alloys, contains numerous interfaces and domains. Functional properties are greatly affected by the interfaces and boundaries between domains. The structural and mechanical properties of nanocrystalline materials was discussed in detail with Vienna's Group (Prof. T. Waitz and Prof. C. Rentenberger) by e-mail and web meeting. At this time, we are preparing to submit these research papers. Also, our research team acquired " Promotion of Joint International Research (International Collaborative Research) of KAKENHI" to collaborate the research more strongly. A doctoral student of Matsuda's group stayed in University of Vienna for one month to research the shape memory alloy with Vienna's Group.

***Publications collaborated with unit members***


[1] Jann-Erik Brandenburg, Luis A. Barrales-Mora, Sadahiro Tsurekawa, Dmitri A. Molodov, *"Dynamic behavior of grain boundaries with misorientations in the vicinity of Σ3 coherent and incoherent twin boundaries in Al bicrystals"*, Acta Materialia, 259, (2023) 119272. (DOI: https://doi.org/10.1016/j.actamat.2023.119272)


***List of awards, grants, and patents***

[1] M. Matsuda: Promotion of Joint International Research (International Collaborative Research) of KAKENHI, "*Characteristic control based on quantitative evaluation of nano-defect and defect-induced strain field in functional materials*", Grant Number 23KK0087 (from FY2023 to FY2027).

[2] S. Tsurekawa: Grant-in-Aid for Scientific Research (B), "*Grain boundary – dislocation interactions under chemical and physical reaction fields associated with grain boundary segregation*", Grant Number 20H001760 (from FY2022 to FY2025).

[3] S. Tsurekawa: The Iron and Steel Institute of Japan (ISIJ) Research Project, "*Approach of grain boundary engineering for achieving high- permance steels*" (from FY2023 to FY2025).

| | | | |
|---|---|---|---|
| No. 2-5-13 | Structure and Dynamics of Materials Using Quantum Beams and Data-Driven Sciences | |  |
| **Cluster Coordinator** | | | |
| Name | Ichiro AKAI | | |
| Affiliation,<br>E-mail | Institute of Industrial Nanomaterials（IINa）<br>Email: iakai@kumamoto-u.ac.jp | Title | Professor |
| Research Field | Advanced materials / Data science and AI | | |

| **Cluster Members** | |
|---|---|
| Name | Affiliation/Title |
| Marc DE BOISSIEU | SIMaP, CNRS, Université Grenoble Alpes, France<br>Director |
| Matthieu MICOULAUT | Sorbonne Université, France<br>Professor |
| Anita ZEITLER | Department of Physics, University of Bath, UK<br>Lecturer |
| László PUSZTAI | HUN-REN Wigner Research Centre for Physics, Hungary/ IROAST<br>Scientific Advisor, IROAST Distinguished Professor |
| Masaru ANIYA | FAST, Kumamoto University<br>Professor |
| Masahiro HARA | FAST, Kumamoto University<br>Associate Professor |
| Yoichi NAKAJIMA | FAST, Kumamoto University<br>Associate Professor |
| Shinya HOSOKAWA | IINa, Kumamoto University<br>Project Professor |

**[Details of activities]**

## 1. Research outline and its perspective

This research group aims to investigate the structure and dynamics of materials using quantum beam facilities in combination with data-driven sciences and computer simulations. Recent developments in quantum beam facilities, such as synchrotron radiation, x-ray free-electron laser, and intense neutron sources, have led to remarkable progress in the quality of experimental data. In conjunction with them, new varieties of data sets appear, such as two-dimensional images, etc., and the corresponding data volumes explosively increase. The present task for researchers is how to extract scientifically valuable information from the experimental data of huge size in quantity but still insufficient in quality. In this research unit, thus, we carry out state-of-art experiments such as scattering and imaging using quantum beam facilities and analyze the data using, e.g.,

Inverse problem, Bayesian inference with Metropolis' algorithm (reverse Monte Carlo modeling), and others. Furthermore, data-driven science, such as Sparse modeling, is a very promising tool for handling the data. First-principal computer simulations are also indispensable to support the experimental results.

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

Our international collaboration activity has been revived after the lifting of restrictions related to the COVID-19 pandemic in Japan. Professor Pusztai visited IROAST twice in May-Jun and November to discuss collaborative projects with our cluster members. During his stay in November, we had an international seminar titled "Understanding the structure of liquids: from the stone age to artificial intelligence" by Prof. Pusztai in person and online hybrid. In this seminar, we had local faculties and international students onsite at Kumamoto University and collaborators and researchers online from other universities and research institutes (see the photographs below).

Photographs during the 105th IROAST seminar by Prof. Pusztai on 7th November.

Dr. De Boissieu stayed at Kumamoto University in November. During the stay, he discussed research projects with our cluster members and gave an international seminar titled "Thermal conductivity and lattice dynamics in structurally complex materials." We have faculty members and graduate students from Kumamoto University onsite and participants from overseas online in this seminar (see the photographs below).

Photographs during the 108th IROAST seminar by Dr. De Boissieu on 28th November.

Some of our cluster members and their collaborators organized international conferences and met together overseas. Professor Pusztai organized an international meeting, "RMC-8(+1) Conference", held in Budapest, Hungary, 21-23 September. Prof. Hosokawa joined the meeting to give talks on their recent researches based on the quantum beam experimental data with the reverse Monte Carlo modeling simulations. Dr. De Boissieu organized the international conference "The

International Conference on Complex Orders in Condensed Matter" in Evian, France, on 24-29th September. Prof. Hosokawa and Prof. Pusztai were also the organizing committee members at the conference. Prof. Akai visited the University of Camerino, Italy, 1-8 July to improve a collaborative project for data-driven analyses for synchrotron radiation data with Prof. Di Cicco and his colleagues.

These activities of our cluster are leading to research outcomes given in the publication list, including two collaborative works among this cluster members.

## 3. Research plan for the next fiscal year

We will continue to keep and further promote the activity of our research cluster in FY2024. Prof. Pusztai plans to visit IROAST twice in May and late this year. During the stay, Prof. Pusztai will communicate with the cluster members and discuss the joint research work with Dr. Nakajima on high-pressure diffraction measurements on various liquid mixtures and with Prof. Hosokawa on the structure of amorphous materials. A part of joint research involves a joint KAKENHI proposal.

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

1. I. Pethes, L. Pusztai, L. Temleitner, Evolution of the hydrogen-bonded network in methanol-water mixtures upon cooling, *Journal of Molecular Liquids* **386,** 122494, 13 (2023).
2. H. Yamada, K. Ohara, S. Hiroi, A. Sakuda, K. Ikeda, T. Ohkubo, K. Nakada, H. Tsukasaki, H. Nakajima, L. Temleitner, L. Pusztai, S. Ariga, A. Matsuo, J. Ding, T. Nakano, T. Kimura, R. Kobayashi, T. Usuki, S. Tahara, K. Amezawa, Y. Tateyama, S. Mori, A. Hayashi, Lithium Ion Transport Environment by Molecular Vibrations in Ion-Conducting Glasses, *Energy And Environmental Materials* Paper: e12612, 10 p. (2024). **scheduled to be issued on May*

## 5. List of awards, grants, and patents

JST CREST: I. Akai, 11,450,000 JPY
Anritsu Corporation: M. Hara, 3,100,000 JPY
JSPS Grant-in-Aid for Scientific Research (C): M. Aniya, 1,040,000 JPY
JSPS Grant-in-Aid for Scientific Research (B): Y. Nakajima, 3,900,000 JPY
JSPS Grant-in-Aid for Transformative Research Areas (A): S. Hosokawa, 3,120,000 JPY
JSPS Grant-in-Aid for Scientific Research (C): S. Hosokawa, 780,000 JPY

| | | | |
|---|---|---|---|
| No, 2-5-14 | Nano-materials for Energy Applications and Environmental Protection | | |
| **Cluster Coordinator** | | | |
| Name | Tetsuya KIDA | | |
| Affiliation,<br>E-mail | Faculty of Advanced Science and Technology<br>Email: tetsuya@kumamoto-u.ac.jp | Title | Professor |
| Research Field | Advanced materials | | |

| **Cluster Members** | |
|---|---|
| Name | Affiliation/Title |
| Armando T. QUITAIN | Headquarters for Admissions and Education, Kumamoto University/ Professor |
| Maria Jose COCERO | Chemical Engineering & Environmental Technology, Universidad de Valladolid Spain/ Professor, *IROAST Visiting Professor* |
| Yusuke INOMATA | Department of Applied Chemistry & Biochemistry, Faculty of Advanced Science and Technology, Kumamoto University/ Assistant Professor |
| Suttichai ASSABUMRUNGRAT | Department of Chemistry Engineering, Faculty of Engineering, Chulalongkorn University/ Professor, *IROAST Visiting Professor* |
| Nicorae BARSAN | The Sensor and Microsystem group at the Institute of Physical and Theoretical Chemistry, University of Tubingen/ Group Head, *IROAST Visiting Professor* |

**[Details of activities]**

## 1. Research outline and its perspective

Our research projects are divided into four categories:

- Synthesis of colloidal quantum dots for optical applications.

Semiconductor nanocrystals called quantum dots (QDs) are expected to be used as phosphors and display materials due to their advantages such as sharp luminescence and high quantum yield (>50%). We have been studying the development of new QDs and their applications. Recently, we have focused on the extremely high luminescence efficiency (100%) of perovskite QDs with a composition of $CsPbX_3$ (X = Cl, Br, I). Furthermore, we discovered that the coexistence of these stabilized perovskite QDs and photochromic (PC) molecules in a solvent can control the on/off of fluorescence upon photo stimulation. We are currently exploring the application of this organic-inorganic hybrid to optical memory.

- Synthesis of oxide nanomaterials for gas sensing.

In recent years, the need for gas sensors has increased as sensors that detect environmental pollutant gases such as $CO_2$, NOx, and SOx have been put to practical use. There are several types of gas sensors, among which semiconductor sensors and solid electrolyte sensors are compact, inexpensive, and highly sensitive sensors. If materials and structures are optimized from the

viewpoint of materials science and catalytic chemistry, they can detect various gases with high sensitivity. Our objective is to establish design guidelines for gas sensors that can detect chemical substances at low ppm concentrations as a new detection technology that enables continuous measurements.

- Electrochemical applications of proton/electron conducting graphene oxide membranes.

A hydrogen energy society is just around the corner, with the nationwide development of hydrogen stations and the commercialization of fuel cell vehicles. In this study, we attempted to produce hydrogen from alcohol using a completely new hydrogen separation membrane based on an electrochemical mechanism, rather than a conventional separation membrane using porous materials. If ethanol derived from biomass can be fed to the electrochemical hydrogen permeation membrane and hydrogen can be produced by the natural oxidation of ethanol, it would be a significant carbon-neutral technology.

- Catalytic conversion of biomass into valuable compounds.

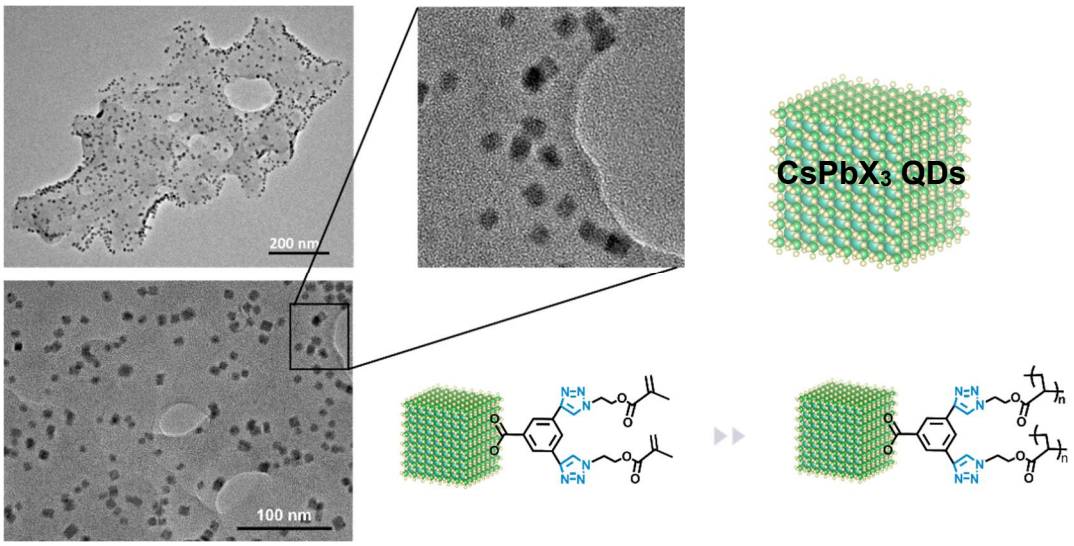
The objective is to produce value-added organic compounds from biomass containing cellulose, protein, and lignin. Cellulose can be separated from cellulosic biomass using sodium hydroxide. Sugars from cellulosic biomass can be used to produce levulinic acid and 5-hydroxymethylfurfural (HMF), which are expected to be renewable chemicals and energy sources in the future. We are currently working on the development of carbon catalysts using graphene oxide (GO), which is obtained by exfoliating graphite sheets. We have found that GO has solid acid properties and excellent microwave absorption, which can promote the hydrolysis of cellulosic biomass to glucose under microwave irradiation. By using graphene-based catalysts, glucose derived from cellulosic biomass can be converted to levulinic acid and HMF.

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

The key achievements include:

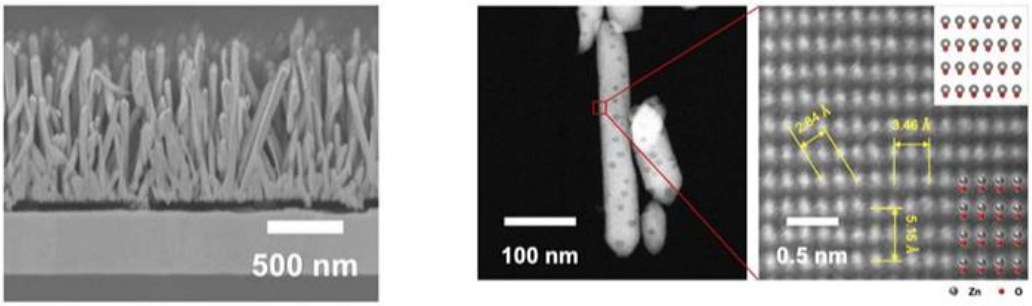
- Synthesis of polymer-coated $CsPbBr_3$ quantum dots.

$CsPbBr_3$ quantum dots are attracting much attention as the highly bright light source. However, their low stability limits the practical uses. By designing and synthesizing surface ligands having azide and alkyne groups, we succeeded in fabricating PMMA polymer-coated $CsPbBr_3$ quantum dots. The synthesized quantum dots showed an excellent stability in polar solvents.



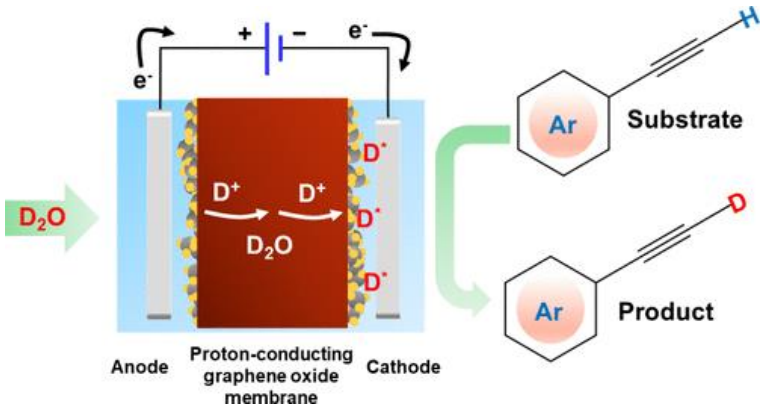
- Development of highly-sensitive gas sensor for volatile organic compounds (VOCs).

Vertically-allied ZnO nanorods showed excellent sensor response to ethanol, acetone, and toluene at ppm concentrations. The detection mechanism was analyzed by in-situ DRIFTS measurements.




- Development of GO-based membrane reactors for the deuteration of organic compounds.

The deuteration of organic molecules is considerably important in organic and medicinal chemistry. An electrochemical membrane reactor using proton-conducting graphene oxide (GO) nanosheets was developed to synthesize valuable deuterium-labeled products via an efficient hydrogen-to-deuterium (H/D) exchange under mild conditions at ambient temperature and atmospheric pressure.




## 3. Research plan for the next year

- Development of photocapacitors using quantum dots and polyoxometallates for solar energy storage.
- Analysis of gas sensing mechanism of oxide nanomaterials by operando measurements.
- Development of GO-based membrane reactors for the deuteration of various organic chemicals and deuterium gas production.
- Design of active catalysts for hydrogenation of organic molecules to produce vale-added chemicals.

## 4. List of grants

- MEXT/JSPS KAKENHI Grant-in-Aid for Scientific Research（B）, “ON/OFF Emission Switching of Perovskite Quantum Dots”, 2020.4~2024.3, 17,680,000-yen, PI: Tetsuya KIDA
- MEXT/JSPS KAKENHI Fund for the Promotion of Joint International Research (Fostering Joint International Research (B)), “Design of highly sensitive gas recognition interfaces using 1D/2D nanomaterials”, 2020.11~2025.3, 18,720,000-yen, PI: Tetsuya KIDA
- JSPS Bilateral joint research project (LIPI Indonesia), “Development of electrochemical devices and membrane reactors based on proton conducting carbon nanosheet membranes”,

2022.4~2024.3, 3,900,000-yen, PI: Tetsuya KIDA

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

(1) T. Shinkai, J.K.C.N. Agutaya, B. Manna, M. Boepple, M. Iwai, K. Masumoto, K. Koga, K. Kawanami, Y. Nakamura, A. T. Quitain, K. Suematsu, Y. Inomata, N. Barsan**, **T. Kida***, Ethanol Sensing Mechanism of ZnO Nanorods Revealed By DRIFT Spectroscopy and DFT Calculations, ***Journal of Materials Chemistry A***, 12, 7564-7576 (2024). ***IROAST Visiting Professor* (＊Co-authored Paper with IROAST Visiting Professor) **Scheduled in issued in April 2024*

(2) I Sahroni, T Kodama, MS Ahmad, T Nakahara, Y Inomata, **T. Kida***, Graphene Oxide Membrane Reactor for Electrochemical Deuteration Reactions, ***Nano Letters***, 24, 12, 3590–3597 (2024).

(3) M. S. Ahmad, Y. Inomata, **T. Kida***, Energy Application of Graphene Based Membrane: Hydrogen Separation, ***The Chemical Record***, e202300163 (2023).

(4) M. Ashraf, R. Ali, N. Ullah, M. S. Ahmad, **T. Kida**, S. Wooh, W. Tremel, U. Schwingenschlögl, M. N. Tahir, Bandgap Engineering of Melon Using Highly Reduced Graphene Oxide for Enhanced Photoelectrochemical Hydrogen Evolution, ***Advanced Materials***, 2301342 (2023).

(5) K. Sonda, T. Kodama, M.D. Wea Siga, K. Masumoto, M. Iwai, M. Fadil, M. S. Ahmad, J. K.C. Agutaya, Y. Inomata, A. T Quitain, A. Hardiansyah, **T. Kida***, Selective Detection of CO Using Proton-Conducting Graphene Oxide Membranes with Pt-Doped $SnO_2$ Electrocatalysts: Mechanistic Study by Operando DRIFTS, ***ACS Applied Materials and Interfaces,*** 15, 45, 52724–52734 (2023).

(6) Y. Tano, M.S. Ahmad, Y. Watase, T. Tsugawa, S. Takase, **Y. Inomata**, K. Hatakeyama, S. Ida, A.T. Quitain, Y. Shimizu, **T. Kida***, Enhancement of Formic Acid Formation by Nitrogen-Doped Graphene Oxide Nanosheets Decorated with Sn Nanoparticles in Electrochemical $CO_2$ Reduction, ***Sustainable Energy and Fuels***, 7, 3964-3971 (2023).

(7) S. Ullah, S. Wang, M.S. Ahmad, H.M.A. Sharif, Q. Liu, **T. Kida**, A. Shafique, M. Ur Rehman, G. Wang, J. Qiu, Investigating the Role Of Oxygen Vacancies In Metal Oxide For Enhanced Electrochemical Reduction Of $NO^{3-}$ To $NH_3$: Mechanistic Insights, ***Inorganic Chemistry Frontiers***, 10 (22), 6440-6488 (2023).

(8) M.S. Ahmad, Y. Nagata, K. Masumoto, Y. Inomata, K. Hatakeyama, A. T. Quitain, A. Shotipruk, **T. Kida***, Manganese Doped Graphene Oxide: Selective Hydrogenation Catalyst for Converting 5-Hydroxymethyl Furfural to 5-Methyl Furfural, ***Molecular Catalysis***, 553, 113787 (2024).

(9) Hapid, Abdul; Zullaikah, Siti; Mahfud, Adji; Kawigraha, Adji; Sudiyanto, Yanto; Nareswari, Ratika Benita; Quitain, Armando T. Oxidation of sulfide mineral and metal extraction analysis in the microwave-assisted roasting pretreatment of refractory gold ore, ***Arabian Journal of Chemistry***, 17 (1), 105447 (2024)

＊Co-authored papers with internship students accepted under the IROAST Internship Program

(1) A. Hardiansyah*, G.M.A. Saputra, H. Hikmat, Y.E. Kusfarida, N.L.W. Septiani, A. Randy, A. Hermawan, B. Yuliarto, T.Y. Liu, T. Kida, Electrochemical Evaluation of Magnetic Reduced Graphene Oxide Nanosheet‐Modified Glassy Carbon Electrode On Dopamine Electrochemical Sensor For Parkinson's Diagnostic Application, ***Journal of the Chinese Chemical Society***, 70 (8), 1665-1682 (2023). **Internship student (2020.1.6-2020.2.28)*

(2) A. Hardiansyah*, G.K. Sunnardianto, S.A. Pradanawati, D.M. Aditya, T. Kida, T.Y. Liu, Investigating the Impact of Nitrogen-Doping On the Characteristics and Performance of Reduced Graphene Oxide for Lithium-Ion Batteries Anode Through Experimental and Theoretical Study, ***Materials Today Communications***, 38, 107740 (2023). **Internship student (2020.1.6-2020.2.28)*

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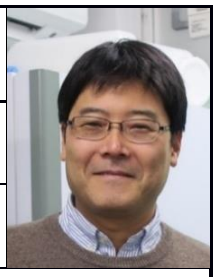
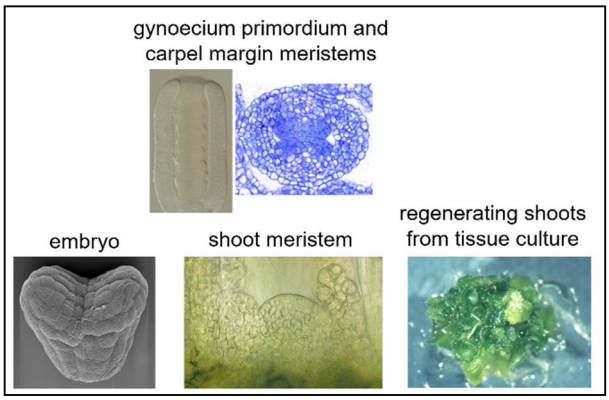
| No. 2-5-15 | Plant Stem Cells and Regeneration | |  |
| **Cluster Coordinator** | | | |
| Name | Mitsuhiro AIDA | | |
| Affiliation,<br>E-mail | Faculty of Advanced Science and Technology<br>m-aida@kumamoto-u.ac.jp | Title | Professor |
| Research Field | Environmental bioscience | | |
| **Cluster Members** | | | |
| Name | Affiliation/Title | | |
| Yoshihisa IKEDA | Centre of the Region Haná for Biotechnological and Agricultural Research, Czech Advanced Technology and Research Institute (CATRIN), Palacký University/Junior Researcher | | |
| Stefan<br>DE FOLTER | Unidad de Genómica Avanzada (LANGEBIO), Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional (CINVESTAV-IPN), Guanajuato, México | | |
| Jose Irepan<br>REYES-OLALDE | Universidad Estatal del Valle de Toluca, Ocoyoacac Edo. Mex. Mexico | | |

**[Details of activities]**

## 1. Research outline and its perspective




Plants possess a remarkable ability to regenerate, wherein single differentiated cells can be reprogrammed to develop into a whole plant. This process involves the de novo formation of stem cell tissue known as the meristem and depends on the actions of two plant hormones: cytokinin and auxin. Within this research cluster, we aim to explore the regulatory mechanisms of gene cascades dictated by a set of transcription factors involved in tissue regeneration, using Arabidopsis thaliana as a model plant. Additionally, we will investigate related developmental processes such as embryogenesis and gynoecium development, which respectively form the embryonic shoot meristem and carpel margin meristems. Understanding these processes contributes to our broader knowledge of plant developmental biology and potential applications in agriculture.

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

The formation of embryonic shoot meristems is a crucial process that establishes a stem cell population responsible for generating the entire shoot system of a plant. The mechanisms regulating this process involve common factors responsible for shoot regeneration. For

instance, a shared set of transcription factors, including WUS, STM, and CUC proteins, is essential for shoot meristem formation in both embryogenesis and regeneration. Moreover, a high cytokinin-to-auxin ratio promotes shoot formation in both developmental contexts.

During embryonic shoot meristem formation, our previous research using the cytokinin response reporter TCSn has revealed a gradual development of the cytokinin response in the presumptive shoot meristem. This increase in cytokinin response depends on the activities of the transcription factors CUC1, CUC2, and CUC3. This year, our focus was on examining the expression of genes encoding cytokinin signaling and biosynthesis. We observed the expression of a receptor gene in developing shoot meristems from early embryogenesis, while genes encoding cytokinin activating enzymes were expressed in surrounding regions of the prospective shoot meristem. These results indicate that cytokinin acts as a mobile signal to establish the shoot meristem. Furthermore, our results enhance understanding of cytokinin's role as a key regulatory molecule in plant development.

In the context of gynoecium development, we found that the response to exogenous cytokinin required the activities of CUC1 and CUC2 but not CUC3. Additionally, CUC1 activates some cytokinin signaling components, including the receptor gene and a transcription factor gene mediating cytokinin response, possibly through binding their upstream regulatory sequences. Our findings suggest that the mechanisms for establishing cytokinin signaling are regulated by a partially overlapping set of transcription factors compared to those in embryogenesis.

## 3. Research plan for the next year

Our research has highlighted the importance of the transcription factors CUC1 and CUC2 in establishing cytokinin response in meristematic tissues during embryonic shoot meristem formation and gynoecium development. In the upcoming year, we plan to assess the functional importance of cytokinin signaling components downstream of the *CUC* genes. This will involve the forced expression of the identified cytokinin signaling genes in loss-of-function mutants of the CUC genes, allowing us to examine whether the defects in embryonic shoot meristem formation and in gynoecium development of the mutants can be rescued. Additionally, we will test whether the expression of these cytokinin signaling components depends on the *CUC* gene activities both in embryo and gynoecium development. By dissecting these pathways, we aim to further elucidate the molecular interactions essential for plant developmental processes.

## 4. List of awards, grants, and patents

N/A

## 5. List of journal papers

Reyes-Olalde IJ, Aida M, de Folter S (2023). An evo-devo view of the gynoecium. J Exp Bot erad135. doi: 10.1093/jxb/erad135.