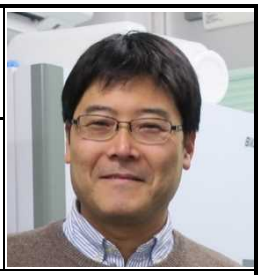
2-1. IROAST Tenure-track Professor and Associate Professors

No.	Name	Project Title
2-1-1	**Mitsuhiro AIDA** (-June, 2022)	Plant Developmental Biology
2-1-2	**Gaochuang CAI**	Design for structural safety and sustainability (DfS3)
2-1-3	**Masahiko FURUTANI**	Adaptive response of plant roots to abiotic and biotic stresses
2-1-4	**Hiroki MATSUO**	Development of polar materials for energy storage and conversion applications
2-1-5	**Zhongyue ZHANG**	Exploring the electronic structure evolution in the electrochemistry process in 2D MOFs.

No.1-1	Plant Developmental Biology			
Name	Mitsuhiro AIDA	Title	Professor	
Affiliation	IROAST (-June 30, 2022) Email: m-aida@kumamoto-u.ac.jp			
Research Field	Environmental bioscience			

Details of activities

1. Research outline and its perspective

Our research aim is to elucidate genetic mechanisms that regulate the activity of shoot meristem, a group of dividing cells responsible for production of plant aerial organs, such as leaves, stems, and floral organs (Figure 1). In dicotyledonous plants, the shoot meristem is initially formed during embryogenesis in a boundary region between the two cotyledon primordia, and after germination, it maintains a group of stem cells at its center and continuously provides new cells that give rise to shoot organs from its periphery.

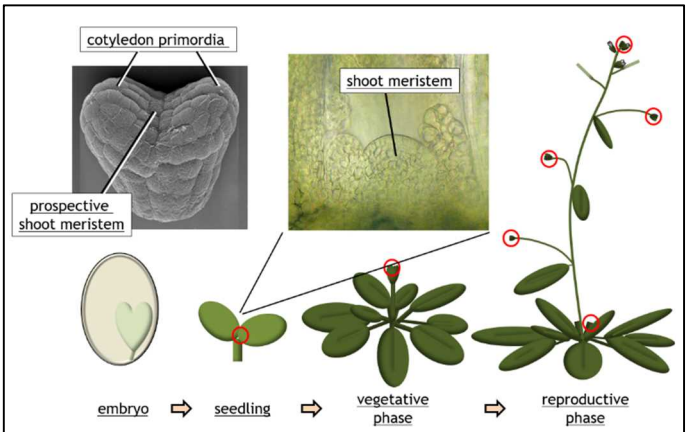


Figure 1. Plant lifecycle and shoot meristem.

2. Research progress and results in the fiscal year

Embryonic shoot meristem and cotyledon formation requires coordinated activities of the phytohormone auxin, whose distribution is determined by the biosynthesis, polar transport, and perception machinery. This year we analyzed how this machinery is regulated in the embryonic apical region, where the shoot meristem and cotyledon primordia arise. The *CUP-SHAPED COTYOLEDON* (*CUC*) genes *CUC1*, *CUC2*, and *CUC3*, which encode transcription factors involved in shoot meristem formation and cotyledon separation, are required for proper distribution of auxin response peaks in the apical region. Quantitative RT-PCR and reporter gene analysis showed that loss of function mutations in these genes caused significant reduction in the expression of the *YUCCA* genes *YUC1* and *YUC4* (Figure 2), each encoding an enzyme that catalyzes a rate-limiting step in auxin biosynthesis, indicating an important role for the *CUC* genes in promoting auxin biosynthesis in the apical region. The contribution of the *SHOOT MERISTEMLESS* (*STM*) gene, which encodes a KNOX-I transcription factor acting downstream of the *CUC* genes in shoot meristem formation, was less obvious because mutations in this gene did not significantly alter *YUC1* expression. Together, our results indicate that the *CUC* genes are involved in establishing proper distribution of auxin response peaks partially through activating the auxin biosynthesis in the cotyledon boundary region. and this regulation is independent of *STM* at least for *YUC1*. We also analyzed the effects of the *CUC* genes on auxin transport and pharmacological experiments suggested that these genes were also important for promoting auxin transport

activities. Considering that subcellar localization of the auxin transporter protein PIN1 is oriented so that it directs auxin from the boundary region to the tips of cotyledon primordia, we speculate that the role of *CUC* genes in auxin distribution is to promote polar transport of auxin out of its source, which itself requires the *CUC* gene activity.

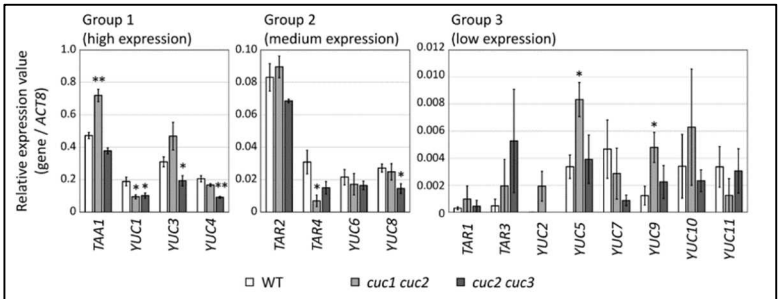


Figure 2. Expression of auxin biosynthetic genes in embryos (Yamada et al 2022, Plant Biotechnol).

3. Research plan for the next year
   To further understand the mechanisms regulating auxin distribution during embryogenesis, we are now studying the effects of the *CUC* genes on genes involved in auxin perception. In addition, investing the combined effects of auxin signaling and the *STM* gene, which are both under the control of the common master regulators encoded by the *CUC* genes, to understand how the activities of different pathways for shoot meristem formation are coordinated in the apical region of the embryo. We are also interested in another phytohormone, cytokinin, which is important for maintaining shoot meristem activity. In the shoot meristem, cytokinin response is active in the L3 layer. By using cytokinin response reporter, we will examine how this cytokinin response pattern develops during embryogenesis. We will also examine expression of major components of cytokinin signaling and possible regulatory mechanisms responsible for their expression. These analyses will provide us with novel insights as to how response patterns of auxin and cytokinin are established during embryogenesis, a process that establishes basic body plan of plants.

4. List of awards, grants, and patents
   N/A

5. List of journal papers
   Temman H, Sakamoto T, Ueda M, Sugimoto K, Migihashi M, Yamamoto K, Tsujimoto-Inui Y, Sato H, Shibuta MK, Nishino N, Nakamura T, Shimada H, Taniguchi YY, Takeda S, Aida M, Suzuki T, Seki M, Matsunaga S (2023). Histone deacetylation regulates de novo shoot regeneration. PNAS Nexus 2, pgad002. doi: 10.1093/pnasnexus/pgad002

   Takeda S, Hamamura Y, Sakamoto T, Kimura S, Aida M, Higashiyama T (2022). Non-cell-autonomous regulation of petal initiation in *Arabidopsis thaliana*. Development 149, dev200684. doi: 10.1242/dev.200684

No.1-2	Design for structural safety and sustainability (DfS3)			
Name	Gaochuang CAI	Title	Associate professor	
Affiliation	IROAST Email: cai@kumamoto-u.ac.jp			
Research Field	Strengthening resilience / Advanced materials			

Details of activities

1. Research outline and its perspective

Since October 2021, the following main achievements have been archived,

(1) Experimental investigation of seismic performance of highly resilient RC columns

With debonded high-strength steel bars, we have developed innovative RC beam-column joints with high resilience after being subjected to strong earthquakes. The related calculation models are being developed by analyzing the resistance mechanism and failure modes, and a finite element method analysis. On the other hand, we are also developing the use of ultra-high-performance materials to confine concrete structures to improve the deformation and seismic performance of members, for example, steel tube confined concrete (STCC) members. Based on a series of multiscale experimental investigations of material constitutive and member performance rules, a performance-based seismic design approach for such structures is being developed.

(2) Development of assessment methods of bolted precast RC walls under simulated seismic loads

As a demountable and sustainable structure, a steel-bolted precast RC wall system has been developed and its seismic performance has been experimentally numerically investigated. The construction method of this system is very similar to that of Wall Precast Concrete (PWC) housing in Japan. It has the unique strong and sturdy appearance of reinforced concrete housing and is highly resistant to various disasters. This type of structure is also a form of Design for Deconstruction (DfD) structures, which is of great significance to the sustainable development of future buildings and rapid recovery and reconstruction after disasters.

(3) Development of reinforced CFT columns toward strong earthquake

The seismic behavior of RCFT columns has been experimentally investigated and the design approach of the CFT columns has been proposed including a simplified model for predicting the load-carrying and deformation capacity of the columns.

(4) Seismic performance and key damage control approach of RC frames infilled by masonry walls

The seismic performance of the frames with different filled masonry walls has been experimentally and numerically studied. A capacity and deformation assessment model has been developed for evaluating the seismic behavior of the frames.

2. Research progress and results in the fiscal year (attach 1-2 related photos)

Regarding Part (1) of the research, since the structural laboratory at Kumamoto University has not been used for the past ten years, a lot of finishing equipment will be required from October 2021, and the first phase experiments have been conducted in September 2022. Currently analyzing the data and writing related papers.

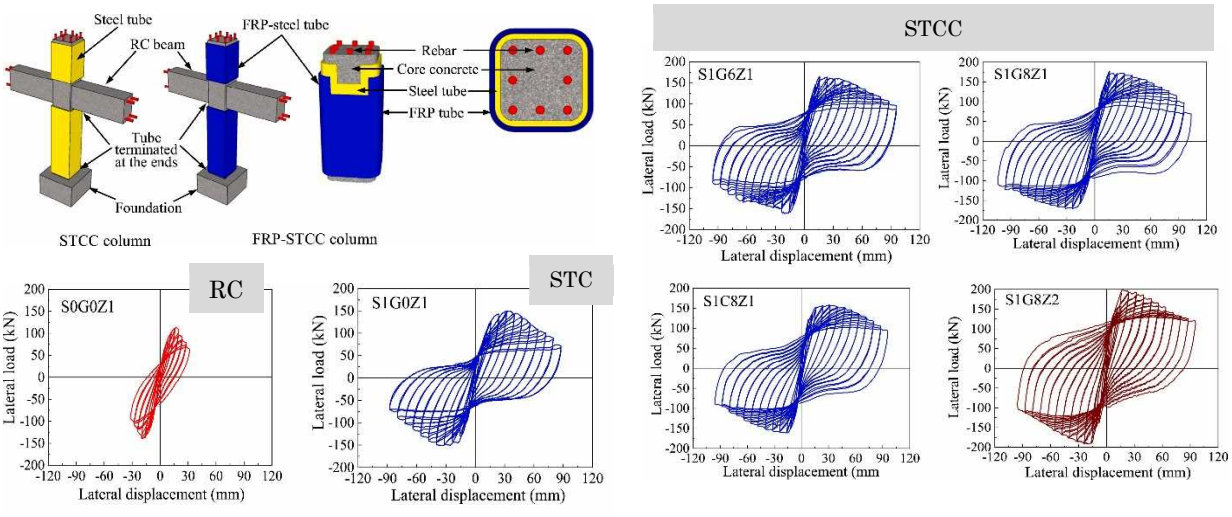


Fig.1 STCC concept and seismic behavior

The research on Parts 2 and 3 is progressing smoothly, and the experimental part has been completed. At present, the experimental data is being analyzed in depth and the design model is being developed, and some papers have been published. Currently, a new paper is being written.

For the fourth part of the research, papers related to experiments and finite element analysis have been published, and another paper has been submitted and is under review.
At present, it is mainly the development of the analysis program of OPENSEES, which is also close to completion.

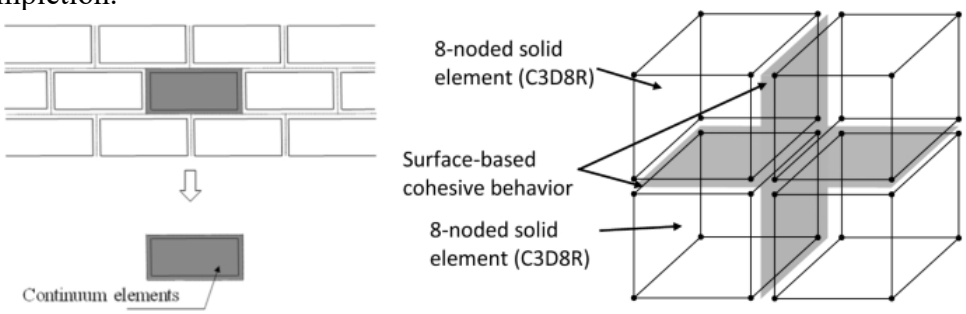


Fig.2 Models of masonry units and the interfaces **a** Masonry portion describing mesoscale model **b** masonry units and surface-based cohesive behavior

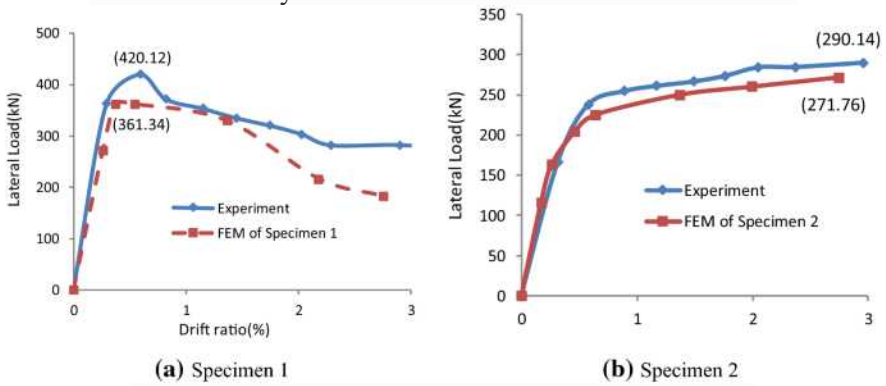


Fig.3 Comparison between test and numerical results

3. Research plan for the next year

According to the current process and results, the following research projects will be conducted next year

(1) Seismic performance and FE analysis of Resilient RC(RRC) shear walls under strong

earthquake
(2) Seismic performance and FE analysis of RRC columns under strong earthquake
(3) Seismic performance and FE analysis of FRP-repaired RRC columns under strong earthquake
(4) Seismic performance and FE analysis of Steel-RC (SRC) columns under strong earthquake
(5) Structural performance and FE analysis of RRC beams under impact loads

4. 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

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

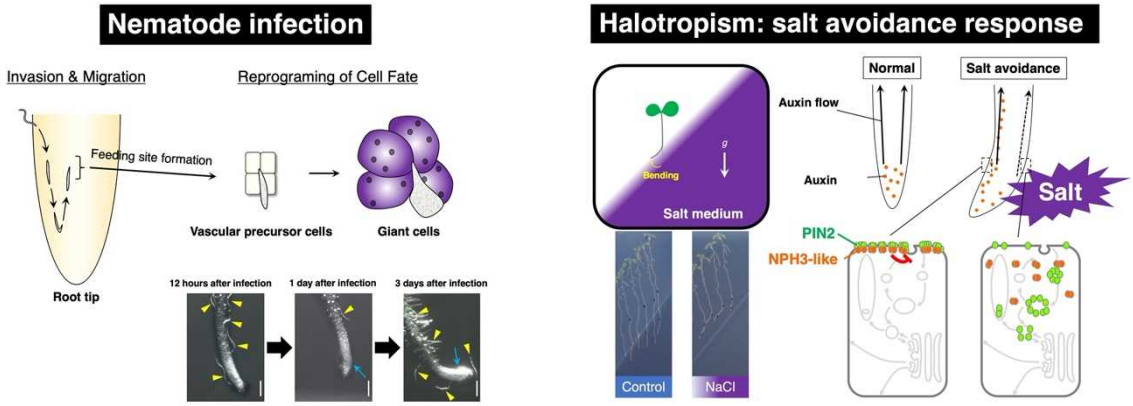
[1] Su, Q., Cai, G.*, Hani, M., Si Larbi, A., & Tsavdaridis, K. D. (2023). Damage control of the masonry infills in RC frames under cyclic loads: a full-scale test study and numerical analyses. *Bulletin of Earthquake Engineering*, *21*(2), 1017-1045. (IF:4.556, Q1)
[2] Wang, Y., & Cai, G.* (2023). Seismic behavior of square concrete columns confined by FRP-steel composite tube. *Journal of Building Engineering*, *65*, 105754. (IF:7.144, Q1) *Issued on April 15, 2023
[3] Zhao, F., Xiong, F., Cai, G.*, Yan, H., Liu, Y., & Larbi, A. S. (2023). Performance and numerical modelling of full-scale demountable bolted PC wall panels subjected to cyclic loading. *Journal of Building Engineering*, *63*, 105556. (IF:7.144, Q1)
[4] Chen, G., Wang, Y., Cai, G.*, Larbi, A. S., Wan, B., & Hao, Q. (2022). Performance and modeling of FRP-steel dually confined reinforced concrete under cyclic axial loading. *Composite Structures*, *300*, 116076. (IF:6.603, Q1)

No.1-3	Adaptive response of plant roots to abiotic and biotic stresses			
Name	Masahiko FURUTANI	Title	Associate Professor	
Affiliation	IROAST Email: ma-furut@kumamoto-u.ac.jp			
Research Field	Environmental bioscience			

[Details of activities]

1. Research outline and its perspective

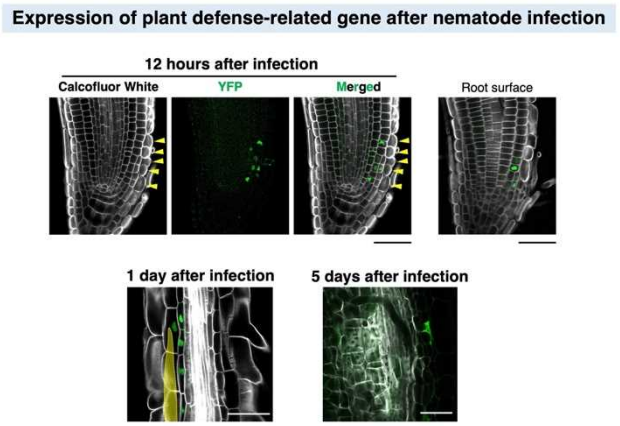
In this project, our group investigates the molecular mechanisms of adaptive response of plant roots to root-knot nematode infection and high salinity using physiological, genetic, biochemical, and structural biological approaches. In addition, based on the knowledge of the molecular mechanisms, we are going to establish nematode infection and salt damage control methods by generating genome-editing plants and developing agricultural chemicals.



2. Research progress and results in the fiscal year

(a) Nematode infection

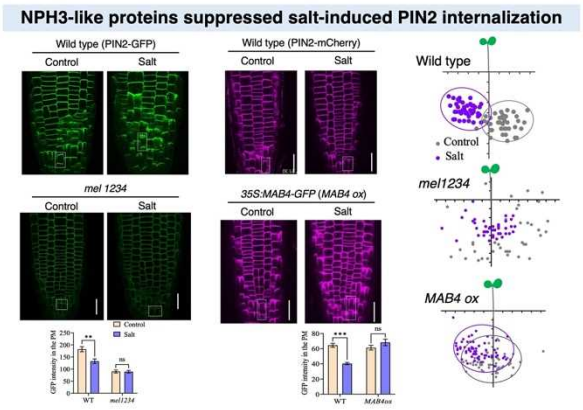
At the early stage of root-knot nematode infection, nematodes invade into host roots by digesting plant cell walls and migrate to precursor vascular cells. We have identified several genes that were upregulated specifically in the early step of nematode infection. Defense-related genes were transiently upregulated after nematode infection. The expressions of these genes were detected at the nematode invasion sites (12 hours after nematode infection). At 2 and 3 days after nematode infection, these genes were upregulated in nematode surrounding cells. However, at 5 days after nematode infection, the expression of these genes disappeared. These results indicate that plant defense response against nematode infection occurs at the early stage and later plant defense is abolished after nematode migration to vascular precursor cells, suggesting that abolishment of plant defense against nematode infection could be induced by



nematode effectors injected into vascular precursor cells.

(b) Halotropism

Roots bend away from high salinity through the control of polar auxin transport in root tips. We found that salt-induced PIN2 internalization (endocytosis from the plasma membrane) in the lateral root cap cells contribute to salt avoidance response, halotropism. In addition, NPH3-like proteins, key negative regulators of PIN endocytosis, identified by our group previously, were found to be dissociated from the plasma membrane. This salt-dependent dissociation from the plasma membrane is required for PIN2 internalization in high salinity. These findings indicate that salt responsive dissociation of NPH3-like proteins from the plasma membrane would mediate salt signaling in halotopism.



3. Research plan for the next year

(a) Nematode infection

This year, we are going to investigate the molecular mechanism of the termination of plant defense after nematode arrival at the vascular precursor cells. At first, we are going to compare the transient expression of plant defense genes induced by nematode infection with expression of defense genes induced by bacterial elicitors such as flagellin fragment (Flg22) and chitins. Previously, bacterial elicitors have been reported to induce prolonged expression of plant defense genes, not transient expression. If we could find the difference of expression of plant defense genes between nematode infection and bacterial elicitor, this would suggest the presence of effectors that could suppress plant defense. In fact, several nematode effectors were already reported to suppress plant defense against bacterial infection and bacterial elicitors. We are going to investigate the role of these nematode effectors in the termination of plant defense against nematode infection to elucidate the interaction between plant and nematode from the viewpoint from plant defense.

(b) Halotropism

We are going to investigate the molecular mechanism of the dissociation of NPH3-like proteins from the plasma membrane in response to high salinity. We previously identified a point mutation (Y409F) in the MAB4, a member of NPH3-like proteins, proteins that could stabilize its localization. We will examine the effect of this mutation on salt-induced dissociation of NPH3-like proteins including MAB4 from the plasma membrane and salt avoidance response. In addition, the mechanism by which the Y409F mutation stabilizes MAB4 localization in the plasma membrane will be investigated. Wild-type MAB4 and mutated MAB4 Y409F will be purified from E. coli and the lipid-protein overlay assay will be performed using the purified MAB4 proteins.

4. List of awards, grants, and patents

Principal Investigator (PI)

1. National Natural Science Foundation of China (NSFC), General Program

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

Man Gao, Emmanuel Aguilar, Borja Garnelo Gómez, Laura Medina-Puche, Pengfei Fan, Irene Ontiveros, Shaojun Pan, Huang Tan, Edda von Roepenack-Lahaye, Na Chen, Xiao-Wei Wang, David C Baulcombe, Eduardo R Bejarano, Juan Antonio Díaz-Pendón, Masahiko Furutani, Miyo Terao Morita, Rosa Lozano-Durán. (2022) A plant virus causes symptoms through the deployment of a host-mimicking protein domain to attract the insect vector. bioRxiv. DOI: 10.1101/2022.12.16.520777

No.1-4	Development of polar materials for energy storage and conversion applications			
Name	Hiroki MATSUO	Title	Associate Professor	
Affiliation	IROAST Email: matsuo_h@cs.kumamoto-u.ac.jp			
Research Field	Advanced materials			

1. Research outline and its perspective

We have developed sodium niobate ($NaNbO_3$)-based antiferroelectric ceramics for energy storage applications. Our Ca-modified $NaNbO_3$ ceramics exhibited a clear double polarization (P)-electric field (E) hysteresis loop arising from an E-induced reversible phase transition between antiferroelectric (AFE) to ferroelectric (FE) phases (Fig. 1). The reversible phase transition was confirmed by X-ray diffraction measurements for the ceramic samples before and after the application of E. We consider that chemically induced compressive strain by Ca doping stabilizes the AFE phase of $NaNbO_3$.

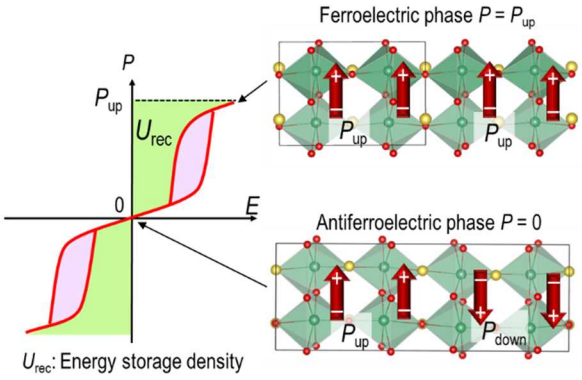


Fig. 1. Typical double P-E hysteresis loop of antiferroelectric materials showing E-induced reversible phase transition between antiferroelectric and ferroelectric phases.

2. Research progress and results

Antiferroelectrics are potential materials for energy storage ceramic capacitors. They have antipolar ordering of constituent atoms at $E = 0$ as shown in Fig. 1, and the resultant net P is zero because P_{up} and P_{down} cancel each other out. In principle, by the application of E, they can exhibit large polarization change associated with a reversible phase transition between AFE and FE phases, and thereby exhibit large recoverable energy density (U_{rec}).

$NaNbO_3$ is a representative lead-free perovskite oxide having antipolar ordering. However, an irreversible phase transition from the AFE to the FE phase usually takes place, and a double P-E hysteresis loop, which delivers high U_{rec}, does not appear. In this term, we investigated the properties of Ca-modified $NaNbO_3$ $(Na_{1-2x}Ca_xV_x)NbO_3$ (V: Na-site vacancy) ceramics[Fig. 2(a)], in which Na^+ site is partially substituted by Ca^{2+} accompanied by the formation of V [Fig. 2(b)]. We found the volume of perovskite unit cell of Ca-modified $NaNbO_3$ decreases with increasing Ca content x because of the introduction of compressive chemical pressure. While ceramics with $x = 0.005$ showed a single P-E hysteresis loop indicating the E-induced irreversible phase transition from the AFE to FE phase, ceramics with an optimal x of 0.10 showed a clear double P-E hysteresis loop arising from the reversible E-induced phase transition [Fig. 2(c)]. The reversible phase transition for $x = 0.10$ is also supported by the result of the current density (J)-E hysteresis loop [Fig. 2(c)] where two current peaks arising from FE to AFE and AFE to FE transitions are observed for both positive and negative E sweeps. Further increase in x resulted in marked

stabilization of the antipolar ordering, and the doble *P-E* loops were not obtained probably because threshold electric fields for the phase transition exceeded break-down fields of the samples. We consider that the introduction of compressive strain by chemical modification is an effective approach to stabilize the AFE phase of $NaNbO_3$-based antiferroelectrics. We have published a paper reporting these results to a preprint server (https://doi.org/10.21203/rs.3.rs-2558019/v1).

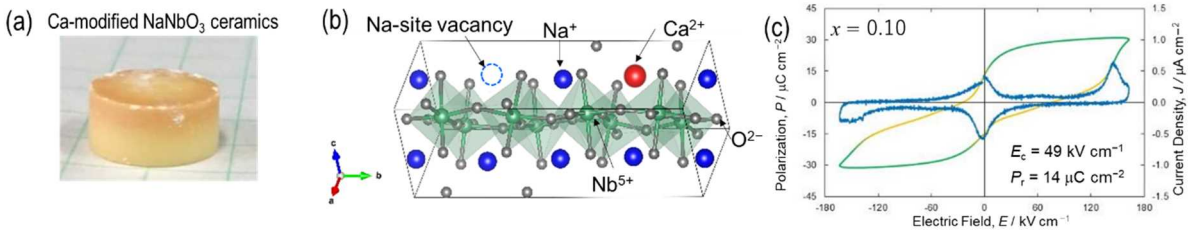


Fig. 2(a) Photograph of Ca-modified $NaNbO_3$ ceramics. (b) Crystal structure of antiferroelectric Ca-modified $NaNbO_3$. (c) *P-E* and *J-E* hysteresis loops of ceramics with $x = 0.10$.

3. Research plan for the next year

As for energy-storage ceramic capacitors, we will investigate structural and polarization properties of Ca-modified $NaNbO_3$ ceramics at high temperatures, to clarify the temperature-induced phase transitions of this system. In addition, Bi-based ferrielectric perovskite oxides that also show a large polarization change associated with a reversible phase transition between the ferrielectric and ferroelectric phases will be developed for energy storage applications.

4. List of Awards

1) The 77th Ceramic Society of Japan Awards for Advancements in Ceramic Science and Technology
"Development of Photovoltaic Functions in Perovskite-type Ferroelectric Materials"
Mar. 2023

2) The 13th Korea-Japan Conference on Ferroelectrics (KJC-FE 13) Excellent Presentation Award
"Domain-engineered $BiFeO_3$-based ferroelectrics with high-photocurrent anisotropy for visible-light polarization detection"
Sep. 25^{th}–28^{th}, 2022

5. List of Grants

1) The Asahi Glass Foundation Research Encouragement Grants FY2022, **次世代蓄電デバイスに向けた新規欠陥双極子誘起強誘電体の創製**, April 2022-March, 2023

2) Grant-in-Aid for Early-Career Scientists (The Japan Society for the Promotion of Science), April 2022-March 2023

6. Papers and Presentations

(Papers)

1) Hiroki Matsuo* Masashi Utsunomiya, Yuji Noguchi*
"Utilizing ferrorestorable polarization in energy-storage ceramic capacitors"
NPG Asia Materials 14(1) 80 (2022).
https://doi.org/10.1038/s41427-022-00426-z

2) Yuji Noguchi* and Hiroki Matsuo

"Origin of Ferroelectricity in BiFeO3-Based Solid Solutions"
Nanomaterials 12(23) 4163 (2022).
https://doi.org/10.3390/nano12234163

3) Yuji Noguchi*, Hiroki Matsuo
Ferroelectric polarization of tetragonal $BiFeO_3$—an approach from DFT calculations for $BiFeO_3$–$BaTiO_3$ superlattices—
Japanese Journal of Applied Physics 61 SN1002 (2022)
https://doi.org/10.35848/1347-4065/ac7bd2

4) Hiroki Matsuo* and Yuji Noguchi
"High Photocurrent Anisotropy in Domain - Engineered Ferroelectrics for Visible - Light Polarization Detection"
Advanced Optical Materials 10(21) 2201280 (2022)
https://doi.org/10.1002/adom.202201280

5) Hiroki Matsuo* and Yuji Noguchi
"High-quality ferroelectric $B_{0.5}K_{0.5}TiO_3$–$BiFeO_3$ solid-solution single crystals grown under high-pressure oxygen atmosphere"
Applied Physics Express 15(8) 081002 (2022)
https://doi.org/10.35848/1882-0786/ac7eab

(Presentations)
1) Yuji Noguchi and Hiroki Matsuo
"Design of ferroelectric materials for energy storage applications utilizing interaction between defects and polarization"
Annual Meeting 2023 of the Ceramic Society of Japan, Mar. 2023, Yokohama.

2) **(Invited)** Hiroki Matsuo
The 77th Ceramic Society of Japan Awards for Advancements in Ceramic Science and Technology
"Development of Photovoltaic Functions in Perovskite-type Ferroelectric Materials"
Annual Meeting 2023 of the Ceramic Society of Japan, Mar. 2023, Yokohama.

3) Tomoki Sato, Hiroki Matsuo, and Yuji Noguchi
"Photovoltaic effect of Cu-doped $LiNbO_3$ single crystals under visible light"
42nd Meeting on Electronic Materials, Nov. 2022, Yokohama.

4) Shun Fukushima, Hiroki Matsuo, and Yuji Noguchi
"Defect engineering for ferroelectric $BaTiO_3$ for energy storage ceramic capacitors"
42nd Meeting on Electronic Materials, Nov. 2022, Yokohama.

5) Hiroki Matsuo and Yuji Noguchi
"Domain-engineered $BiFeO_3$-base ferroelectric with high-photocurrent anisotropy for visible-light polarization detection"
13th Korea-Japan Conference on Ferroelectrics (KJC-FE13), Sep. 2022, Busan (Virtual)

6) Hiroki Matsuo and Yuji Noguchi
"Ferroelectric Photovoltaic Effect in BiFeO3-based solid-solution thin films with nanodomain structures"
35th Fall Meeting of the Ceramic Society of Japan, Sep. 2022, Tokushima (Virtual).

7) Seiyu Aso, Hiroki Matsuo, and Yuji Noguchi
"Fabrication and characterization of defect-engineered $NaNbO_3$-based antiferroelectric ceramics"
35th Fall Meeting of the Ceramic Society of Japan, Sep. 2022, Tokushima (Virtual).

8) Hiroki Matsuo and Yuji Noguchi
"Enhanced photovoltaic effects in ferroelectric thin films with nanodomains"
15th International Symposium on Ferroic Domains & Micro- to Nano-scopic Structures (ISFD-15), Aug. 2022, Yamanashi.

No.1-5	Exploring the electronic structure evolution in the electrochemistry process in 2D MOFs.			
Name	Zhongyue ZHANG	Title	Associate Professor	
Affiliation	IROAST Email: zhongyuezhang@kumamoto-u.ac.jp			
Research Field	Advanced materials			

Research outline and its perspective

Recently, the study of 2D semiconductive metal-organic frameworks (MOFs) with π-d conjugated structures have demonstrated their outstanding performances in electrochemical cells. In contrast to that, most reports aren't able to provide a solid interpretation to the charge and energy storage mechanism. With the electrochemical magnetometric methods that is developed by Zhang and colleagues, we are able to monitor the electronic and spin structure evolution within a electrochemical reduction step, which not only clarifies the mechanism of these MOFs, but also provides the guideline of developing new 2D molecular materials.

Research progress and results in the fiscal year

Since Prof. Zhang was appointed at Kumamoto University from January 2023, major part of this research is accomplished in Nagoya in 2022. We selected a reported 2D MOF, CuTHQ and carefully monitored the first reduction step with qualitative and quantitative ESR accompanied with magnetic susceptibility measurements. It is revealed that, this MOF evolute from a Cu(II) Kagome lattice to a honeycomb electronic structure in the first reduction, and quantitative ESR suggested the absence of multiple radicals, but the emergence of highly delocalized electrons validated by significantly enhanced temperature independent paramagnetism. This research disproved the mechanism that has been proposed in most articles, which assumed a deeply reduced states of organic ligands and formation of multiple localized radicals. It is illustrated that from the perspective of electronic properties, these 2D conjugated semiconductive MOFs should be considered as 2D solid-state materials, instead of traditional molecular materials with highly localized molecular orbitals. (Fig.1)

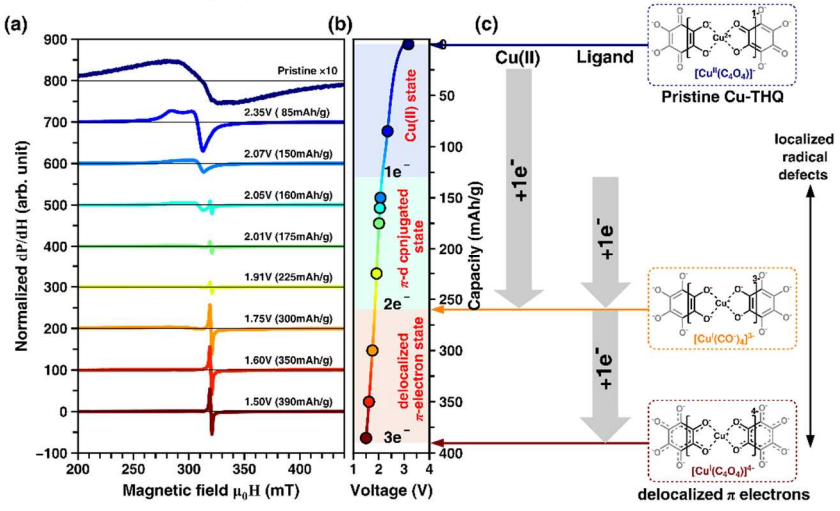


Fig. 1 The evolution of electron and spin states in the first electrochemical reduction step of CuTHQ.

During January to March, Zhang and coworkers in Nagoya University standardized the electrochemical magnetometric approach in details and summarized this method as a protocol which could be used to analyze not only the electrochemistry of 2D MOFs, but also covalent organic frameworks (COFs), conductive polymers and other materials with structural orders. This protocol was accepted as an invited publication in Journal of Visualized Experiments. (Fig.2)

Fig.2 Prof. Zhang visited the Lab of Advanced Materials in Nagoya University for collaborative research.

Research plan for fiscal year 2023

In 2023, we will continue the collaboration with Prof. Zhenfei Liu (Wayne State Univ., USA) and extended the collaboration team with Prof. Jier Huang (Boston College, USA). Prof. Liu is a computational chemist with expertise on the calculation of electronic structures and simulation of transportation properties of materials. Prof. Huang masters the *in situ* and time resolved spectroscopic methods for resolving the charge dynamics in quantum dots, semiconductors and 2D materials. These scientists will be the major collaborator that participate in the international research cluster that is proposed by Zhang.

The proposed research for next fiscal year focuses on the preparation of 2D MOF composites and non-conjugated 2D MOFs with high quality single crystals, and the interpretation of their physical properties. Two targets will be pursued in the next year: (1) the 2D MOF heterojunction type composite materials, which could be achieved by co-condensation of the mixture composed by monodispersed thin film solutions of different MOFs. The potential superstructures that are formed at the interface and interlayer charge transfer across the heterojunction may lead to modification of band structures, Fermi levels and density of states (DOS), which results exotic perturbation to the conductivity or improved stability in electrochemistry. (2) the preparation of non-conjugated 2D MOFs based on triptycene-derivative ligands and the hopping mechanism of conductivity. With the absence of π-d conjugated electronic structure that is commonly seen in planar 2D MOFs, the conductivity of triptycene derived MOFs will originate from the hopping of electrons, which could be characterized by the time-resolved terahertz spectroscopic methods.

Publications:

1. Qi Chen, Zhongyue Zhang,* Kunio Awaga.* Magnetometric Characterization of Intermediates in the Solid-state Electrochemistry of Redox Active Metal-Organic Frameworks (Special Issue of Metal-Organic Frameworks), *J. Vis. Exp.*, Just accepted.