

AIMR

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Research

RESEARCH HIGHLIGHTS

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MESSAGE FROM THE DIRECTOR



Shin-ichi Orimo

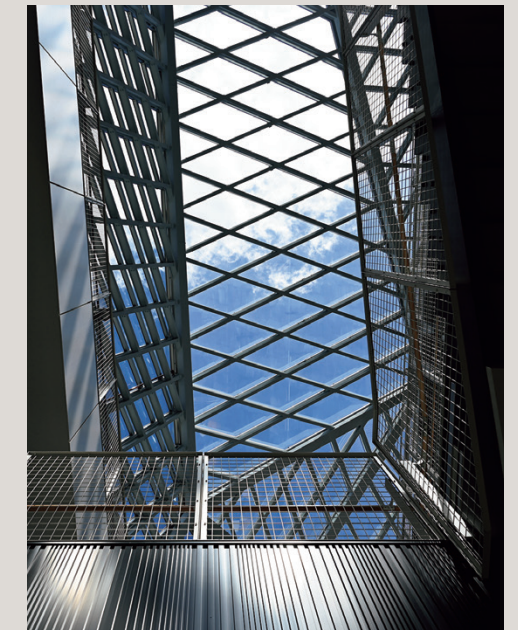
Director
Advanced Institute for Materials Research (AIMR)
Tohoku University



I am delighted that *AIMResearch* 2025 is now being published.

For Tohoku University, 2025 was a pivotal year. Following our official accreditation as a University for International Research Excellence (UREX) the previous year, we have launched full-scale efforts under the Research System Strengthening Plan. Structural reforms are advancing to ensure the University's continuous development as one of the world's leading institutions. Within this framework, there are high expectations for the Advanced Institute for Materials Research (AIMR) to play a central role, utilizing the internationality and leadership we have cultivated up until now.

Amid such developments, AIMR conducted international recruitment in 2025 as part of our efforts to strengthen our research system as a UREX. As a result, we are proud to welcome four new Junior Principal Investigators to our institute. Providing an environment where young researchers can independently pursue challenging research has been one of the guiding principles of AIMR since its foundation.



Furthermore, to realize and accelerate "AI for Materials Science," AIMR's experimental and mathematical research groups are collaborating through "MatSci-DX" to advance the automation and autonomization of materials synthesis and evaluation using robotics. This initiative aims to enhance the approach to research itself by fully incorporating DX and integrating AI, data science, and advanced measurement into functional materials research. These efforts will certainly lift "materials science based on predictions" to a new level and provide an important foundation to pioneer the materials science of the future.

In addition to "Research Highlights," which feature noteworthy papers produced by evolving AIMR, this issue includes "Spotlight" – a section providing overviews of our institutional initiatives and challenges. I hope you will enjoy this new issue, and I look forward to hearing your thoughts and suggestions.

About *AIMResearch*

AIMResearch features articles that provide an accessible introduction to some of the most noteworthy research being done at the Advanced Institute for Materials Research (AIMR), Tohoku University. As one of the world's leading centers for interdisciplinary materials science, AIMR produces hundreds of papers every year. Our "Research Highlights" presents outstanding examples of this research, from a perspective different from those taken in the papers themselves. Alongside these highlights, the "In the Spotlight" series showcases the institute's wide-ranging activities and unique features.

The latest articles are available to read on the institute's website. Readers can also sign up to receive the latest articles to their registered email address.

AIMResearch

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Located on the second floor of the AIMR Main Building, the Common Equipment Room serves as a bustling hub for daily research activities.

Beyond equipment sharing:
AIMR's Common Equipment Room
creates pathways
for research autonomy

website >>>



International researchers entering Japanese academia have historically faced a fundamental challenge: accessing research infrastructure typically required integration into the traditional laboratory (Koza) system, where equipment ownership, research direction, and technical support flow through traditional hierarchical structures. For researchers with independent ideas seeking to establish their own research directions, this model created significant barriers—particularly when language differences complicated equipment operation and maintenance coordination.

The Common Equipment Room at the Advanced Institute for Materials Research (AIMR) at Tohoku University emerged in 2012 as one of the institutional responses to this challenge. More than a shared equipment facility, it has become a critical component in creating alternative pathways for international researchers to integrate into Japanese academia while maintaining research autonomy. The work from Dr. Siraprapha Deebansok—a young researcher originally from Thailand—exemplifies how this infrastructure enables independent research that would otherwise face substantial obstacles.

Professional support, shared access

The Common Equipment Room houses six major research instruments managed by three dedicated technical coordinators who provide comprehensive research technology support. Representative capabilities include a field emission scanning electron microscope for high-resolution surface imaging, a laser Raman spectrometer for molecular characterization, and X-ray diffraction systems for structural analysis. The facility also maintains an atomic force microscope (AFM) that has proven essential for Dr. Deebansok's operando measurement ideas—a project requiring real-time surface characterization during electrochemical operating conditions.

The technical coordinators—all with research backgrounds—provide support that distinguishes the facility from similar university infrastructure. They conduct equipment training, troubleshoot experimental challenges, and assist with research design considerations. Critically, the coordinators work in English, eliminating language barriers that have historically complicated equipment access for international researchers. The facility further developed original pictograms a decade ago to assist researchers unfamiliar with Japanese, demonstrating attention to practical barriers beyond equipment availability.

Creating an alternative

When Prof. Motoko Kotani assumed directorial leadership of AIMR in 2012, she recognized that international research collaboration required more than recruiting foreign researchers—it demanded infrastructure that could accommodate different research cultures and operational expectations. The Common Equipment Room emerged from this recognition.

Japanese research institutions traditionally operated through individual laboratory equipment ownership, with borrowing arrangements coordinated directly between labs. While functional within established research networks, this system created obstacles for newcomers from outside Japan. Finding which laboratory possessed needed equipment, negotiating usage terms, and coordinating schedules presented hurdles even before addressing technical training requirements. For international researchers unfamiliar with institutional networks and facing language barriers during equipment operation, these challenges could significantly slow research progress.

“Our operational model differs fundamentally from the traditional approach where individual laboratories own equipment and coordinate lending arrangements,” explains Dr. Ryotaro Kumashiro, manager of the Common Equipment Room. “When researchers require capabilities unavailable at AIMR, we coordinate access to shared equipment across Tohoku University.”



Custom-designed pictograms help lower language barriers for international researchers unfamiliar with Japanese technical terms.

The Common Equipment Room began modestly, with a single technical staff member coordinating equipment access and managing logistical challenges. The facility gradually acquired instruments through a combination of donations and strategic purchases. Responding to user feedback, it evolved beyond equipment provision to include comprehensive support infrastructure—maintaining tool inventories, stocking various fastener sizes, and developing systems to minimize researcher burden.

By 2015, the Common Equipment Room introduced usage fees to balance operational costs with researcher accessibility, reflecting maturation from experimental initiative to sustainable infrastructure. The staff expanded to three full-time technical coordinators, shifting from primarily coordination work to active equipment management and research support.

Research autonomy in practice

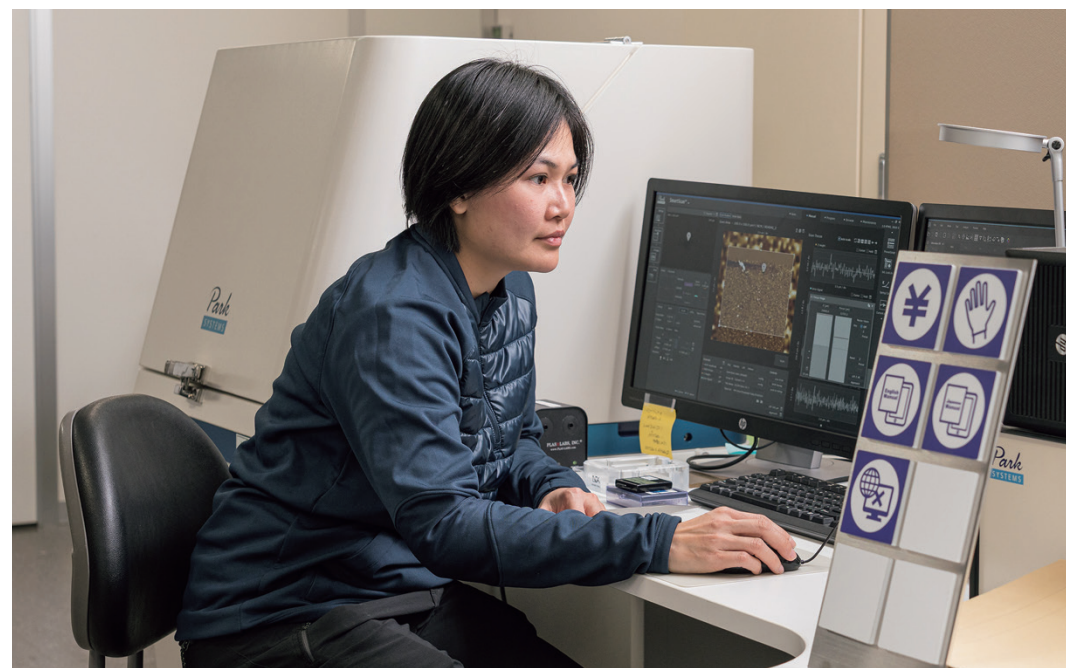
The Common Equipment Room's role in supporting international researchers becomes concrete in Dr. Siraprapha Deebansok's work. Selected through the competitive Core Research Cluster for Materials Science (CRC-MS, directed by Prof. Shin-ichi Orimo), Dr. Deebansok joined AIMR with research ideas requiring sophisticated instrumentation but no affiliation with a traditional laboratory structure possessing such equipment.

The CRC-MS exemplifies the move beyond the Koza system. This inter-departmental organization selects a number of international applicants through competitive proposal review*. Selected researchers pursue independent research directions while receiving extensive organizational support, including career development. One CRC-MS researcher, Dr. Mehrdad Elyasi, was appointed as an AIMR Junior PI in 2025, illustrating how this pathway can enable international researchers to prove concepts through autonomous work rather than vertical laboratory integration.

“The first step of my project aims to prove the operando electrochemical AFM concept: a functional instrument

that can image an electrochemical surface reaction,” explains Dr. Deebansok. Working with collaborators, she designed and built a custom portable electrochemical cell specifically engineered to mount on the Common Equipment Room's AFM. This custom apparatus enables simultaneous surface mapping and mechanical property measurement in liquid environments while offering a level of experimental flexibility—capabilities not available through standard commercial systems under diverse user-defined operating conditions.

“Because I cannot afford an instrument like AFM at this stage of my career, the Common Equipment Room made the project even possible,” Dr. Deebansok notes. As the facility's most frequent AFM user, she progressed from minimal prior AFM experience to designing custom instrumentation around the instrument. Her portable cell has since been tested at other institutions' AFMs, demonstrating reproducible results across different instruments—she is currently preparing these results for publication.



Dr. Siraprapha Deebansok, a frequent user of the facility, leverages its advanced instrumentation to pursue her independent research goals.

Dr. Deebansok's research workflow also illustrates how researchers navigate the broader facility ecosystem beyond AIMR. While the Common Equipment Room provided AFM capabilities, she accessed X-ray photoelectron spectroscopy at a facility in a different building through Tohoku University's Core Facility Center—a university-wide system for coordinating shared equipment access. This integration across departments enabled the comprehensive characterization her research required.

The technical staff's English-language support proved essential throughout. Equipment training, experimental troubleshooting, and technical consultation occurred without language barriers that might otherwise complicate sophisticated custom apparatus development.

* Currently, the five international researchers hired through CRC-MS were selected out of 129 applicants in two recruitment rounds.



Technical coordinators provide essential support, ranging from equipment training to experimental troubleshooting, enabling complex projects to move forward.

Sustaining and expanding the model

While Dr. Deebansok's experience demonstrates the Common Equipment Room fulfilling its core mission, maintaining this level of support presents ongoing challenges.

"More than 10 years have passed since its establishment, and the frequency of troubles has increased, so we are dedicating considerable effort to handling them," Dr. Kumashiro notes. Equipment aging requires

increasing attention as the facility balances high usage rates with measurement reliability and equipment longevity. Booking processes must accommodate frequent users while maintaining access for occasional needs. Maintenance scheduling must minimize research disruption while addressing the reality that near-continuously operating instruments require more frequent servicing.

The growing international researcher population creates sustained demand for meticulous support. The technical coordinator's research backgrounds enable them to engage substantively with experimental design questions rather than merely providing operational instructions. This depth of support—from equipment training through research theme exploration—reduces burden on supervising professors while maintaining research quality. As Dr. Kumashiro emphasizes, "We want to continue to help researchers achieve what they want to do"—a service philosophy that has guided the facility throughout its thirteen-year evolution.

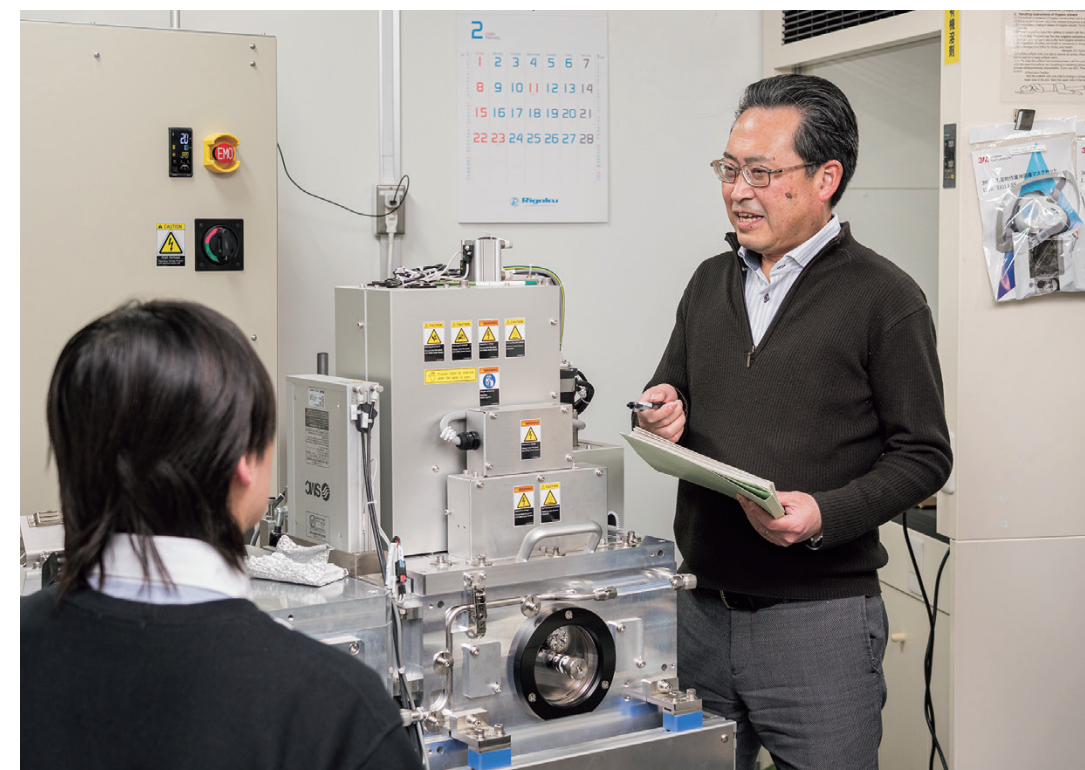
The Common Equipment Room's significance extends beyond AIMR to broader transformations in Japanese research infrastructure. When Tohoku University received designation as Japan's first University for International Research Excellence, the recognition came with substantial funding and a mandate: transition from the traditional Koza system to Principal Investigator-based structures.

This shift makes shared equipment facilities essential. Where the Koza system concentrated equipment ownership within traditional laboratories, PI-based

systems require researchers to access instrumentation across institutional boundaries.

The convergence of multiple initiatives reflects broader transformation in Japanese research infrastructure. Tohoku University's Core Facility Center operates on similar principles of centralized coordination and professional support for shared equipment access. Combined with CRC-MS's competitive pathway and International Research Excellence funding enabling international researcher hiring, these developments have created systemic change. Where international researchers previously faced limited integration pathways outside traditional laboratories, visible alternatives now exist.

Dr. Deebansok's progression from CRC-MS selection to high impact publication preparation demonstrates this pathway in practice. What might appear as merely shared infrastructure becomes, when combined with other institutional changes, a catalyst for transforming academic tradition. International researchers can now contribute to Japanese academia while maintaining research autonomy.



Since the facility's inception, Dr. Ryotaro Kumashiro has been instrumental in cultivating a supportive environment for researchers of all backgrounds.

Carbon nanomaterials:

Machine learning unveils carbon growth mechanism

An AI-driven approach enhances the accuracy and efficiency of carbon deposition modeling

28 April 2025

Corresponding Researchers

Hao Li **Di Zhang**
Principal Investigator Assistant Professor



— Article highlight

Researchers have long sought to model how carbon atoms interact with metal surfaces to form graphene and other carbon materials. Developing this capability would elucidate the growth mechanisms of carbon nanostructures on catalytic substrates, offering new insights into controlling growth, designing novel catalysts and materials, improving energy efficiency, and enhancing scalability.

“A key innovation of this work is its on-the-fly machine-learning training method,” explains Zhang, first author of the article. “The model continuously refines itself by selecting the most relevant atomic configurations. This approach not only enhances predictive accuracy and maintains computational efficiency but also enables the real-time exploration of a wide range of reaction pathways.”

However, conventional computational methods, such as density functional theory (DFT) and kinetic Monte Carlo (KMC) simulations, have struggled to capture the full complexity of these dynamic processes.

Replicating key processes—including carbon diffusion, chain formation, and graphene nucleation—the study revealed that carbon growth on Cu(111) surfaces follows a specific sequence, with adsorbed copper atoms playing a critical role in stabilizing carbon structures. The simulations also demonstrated that oxygen contamination can significantly disrupt graphene nucleation, aligning with experimental observations.

While DFT calculations restrict simulations to small systems due to computational expense, KMC models cannot fully capture the atomic-level dynamics on evolving catalytic surfaces—hindering the development of accurate and predictive models for carbon growth.

By leveraging machine learning, this work establishes a robust theoretical framework for designing metal catalysts to optimize carbon nanostructure synthesis. These findings lay the groundwork for more efficient, large-scale production of graphene and other carbon-based materials, accelerating their adoption in electronics and energy storage.

In a 2024 article, Di Zhang, Hao Li and co-workers at AIMR developed an active machine-learning model to address these challenges¹. The team combined molecular dynamics (MD) and time-stamped force-biased (tf) MC simulations with the gaussian approximation potential to create an efficient approach for simulating carbon deposition on metal surfaces; they also integrated a smooth overlap of atomic positions-based data selection strategy to optimize the training set and improve predictive accuracy.

— A personal insight from Dr. Di Zhang

Which aspect of your study’s results was the most unexpected, and why did it surprise you?

The most unexpected aspect of my study’s results was how efficiently active learning improved the training set for the machine learning force field. Traditional methods rely on random sampling, which often requires large datasets for high accuracy. By combining the MD/tfMC enhanced sampling algorithm with active learning, I streamlined the process, allowing the model

to achieve high-precision predictions with significantly less training data. It was surprising to see how strategic sampling not only reduced data requirements but also maintained—or even improved—accuracy, marking a major advancement over conventional approaches.

Highlight Article

1. Zhang D., Yi P., Lai X., Peng L. and Li H. Active machine learning model for the dynamic simulation and growth mechanisms of carbon on metal surface *Nature Communications* 15, 344 (2024).

Van der Waals bilayers:

Monolayer stiffness stabilizes ferroelectricity above RT

Theoretical model reveals a soft sliding phonon mode that governs the ferroelectric phase transition

26 May 2025

Corresponding Researcher

Ping Tang

Specially Appointed Assistant Professor



website >>>



— Article highlight

Certain two-dimensional (2D) van der Waals-bonded bilayers (e.g., WTe_2 and h-BN) exhibit “sliding ferroelectricity (SF),” where electric polarization arises from specific stacking configurations between monolayers and can be switched by interlayer sliding with an ultra-low energy barrier. This enables energy-efficient switching and enhances material flexibility, making it promising for ultra-thin, low-power ferroelectric devices, such as non-volatile memory and flexible nanoelectronics.

An open question in ferroelectricity research is why SF in WTe_2 and h-BN remains stable well above room temperature (RT) despite their ultra-low electric-polarization switching barriers. Conventional phase transition theories suggest these 2D materials should not exhibit stable ferroelectric order without a substantial barrier, and thus cannot explain the remarkable stability observed in sliding ferroelectrics, where an ultra-low switching barrier has been confirmed experimentally.

In a 2023 article, Ping Tang and Gerrit E.W. Bauer from AIMR developed a thermodynamic model to address this conundrum¹. They proposed that the thermal stability of SF originates from the high in-plane mechanical stiffness of the monolayers, which suppresses thermal fluctuations and reinforces ferroelectric order. Using a mean-field self-consistent phonon approximation, they calculated electric susceptibility and specific heat, quantitatively linking monolayer mechanical properties to ferroelectric stability.

A key finding was the identification of a soft “sliding phonon” mode that governs the phase transition in sliding ferroelectrics. Unlike conventional ferroelectric

phase transitions, where dipole flipping occurs within individual unit cells, the ferroelectric-to-paraelectric transition here is driven by a thermally activated collective sliding of the bilayer, triggered by this soft phonon at the Curie temperature.

“While the ultralow switching barrier from weak interlayer van der Waals forces does not favor stable ferroelectric order, the intralayer stiffness of individual monolayers enhances ferroelectric stability by suppressing the thermally activated collective sliding motion,” says Tang. “This balance between barrier and rigidity explains the high Curie temperatures of WTe_2 and h-BN and distinguishes them from other low-dimensional ferroelectric materials.”

These results demonstrate that the high Curie temperatures of WTe_2 and h-BN bilayers stem from the interplay between their ultra-low switching barriers and significant intralayer rigidity, which prevents rapid thermal depolarization, unlike in other low-dimensional magnetic or ferroelectric materials.

“Our work establishes a unifying theoretical framework for the mechanism underlying the thermal stability of sliding ferroelectricity in van der Waals bilayers,” concludes Tang. “By identifying a soft sliding phonon as the phase transition driver and highlighting the role of monolayer stiffness, we not only elucidated the phase transition mechanism of sliding ferroelectrics but also extended it to structural transitions in non-ferroelectric bilayers. These insights have broad implications for next-generation low-power electronics, spintronics, and bilayer twistrionics.”

— A personal insight from Dr. Ping Tang

What aspect of this research was most rewarding for you, and why?

The most rewarding part was solving a long-standing problem with a simple analytical model. As a theoretical physicist, I aim to understand nature by distilling complexity into its essential components. This work resolved an apparent paradox in van der Waals bilayer ferroelectrics through an intuitive mean-field

approach, revealing that a soft “sliding phonon” mode governs the phase transition. Demonstrating intricate physical phenomena with a minimal yet insightful model was deeply satisfying and reinforced my belief in the power of elegant theoretical frameworks.

Highlight Article

1. Tang P. and Bauer G.E.W. Sliding Phase Transition in Ferroelectric van der Waals Bilayers *Physical Review Letters* 130, 176801 (2023).

Inorganic nanochemistry:

Probing size effects in metal oxide nanoparticles

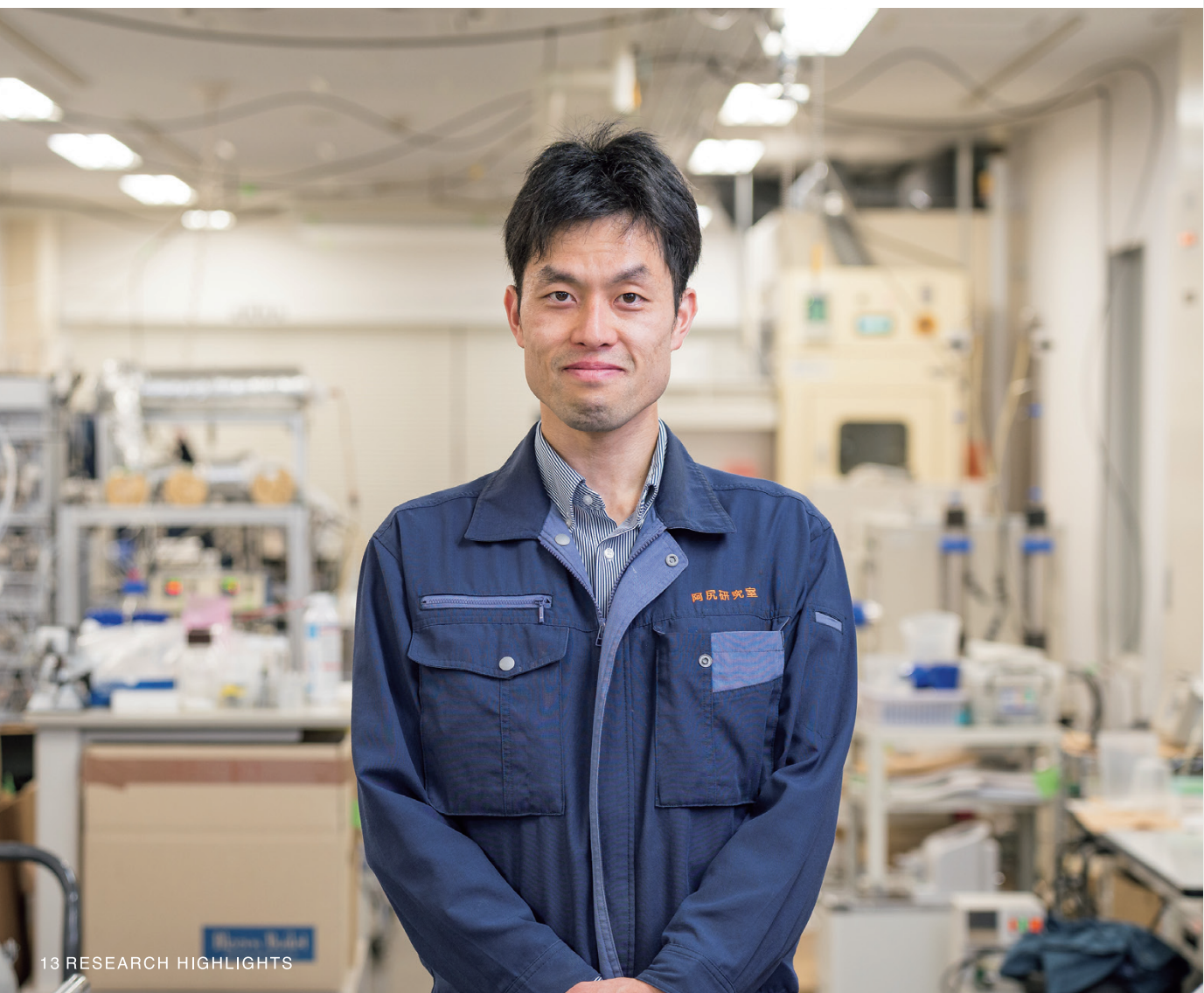
Continuous-flow approach enables ultrasmall CeO₂ synthesis with narrow size distribution

23 June 2025

Corresponding Researcher

Akira Yoko

Associate Professor



website >>>



— Article highlight

Theory and indirect evidence have long predicted that reducing metal oxides to ultrasmall sizes (<5 nm) could lead to unexpected properties driven by structural and electronic changes.

However, unlike in metals and semiconductors, the effects of metal oxide size confinement have yet to be directly investigated, largely due to challenges in synthesizing ultrasmall metal oxide nanoparticles with narrow size distributions and high crystallinity.

“Conventional batch syntheses (where all reagents are mixed, heated, and reacted together in closed vessels under static conditions) often produce particles with broad size distributions and unpredictable properties because of uncontrolled side reactions and unsteady heating,” explains Akira Yoko, a member of an AIMR research team. “Therefore, a different synthetic approach is needed to probe the size effects of metal oxide nanoparticles.”

In a 2024 article, Yoko *et al.* addressed this challenge by developing a continuous-flow supercritical hydrothermal synthesis method that enabled precise control over nanoparticle size down to 1.3 nm¹. The method was designed both to stabilize the nanoparticles using organic modifiers and to control the growth rate through reaction temperature and modifier concentration.

To achieve this, the team combined a flow-reactor process designed for rapid heating, with organometallic chemistry tailored to control how Ce is introduced to the reaction—enabling high conversion rates, fine size control, and reproducible synthesis of ultrasmall CeO₂ nanoparticles.

The study revealed that CeO₂ nanoparticles smaller than 4 nm exhibited dramatic lattice expansion and stacking faults resulting from particle coalescence during early-stage growth. Moreover, the team observed that even without oxygen vacancies, Ce³⁺ electronic states emerged due to oxygen disordering—a previously unreported phenomenon.

“Our findings are significant because they demonstrate that the structural distortion and electron localization observed in CeO₂ nanoparticles arise from nanoscale effects rather than conventional defect chemistry,” says Yoko. “These results open new possibilities for tuning the electronic and catalytic properties of metal oxides by controlling size and growth dynamics at the atomic scale.”

— A personal insight from Dr. Akira Yoko

What result or discovery surprised you the most, and why?

We started out trying to understand the organic modification mechanism in hydrothermal reactions. That led us to study organic–inorganic complex chemistry and eventually improve the precursor for continuous-flow synthesis. What surprised us was that, by precisely controlling the reaction time—down to 40 milliseconds—we could continuously synthesize ultrasmall metal oxides, even smaller than 2

nanometers, which we didn’t expect. The biggest surprise was that these tiny particles had high crystallinity but still showed large structural distortion that caused electron localization without needing lots of oxygen vacancies. We also explored fusion growth, which was fascinating. This method should work for many other metal oxides.

Highlight Article

1. Yoko A., Omura Y., Ninomiya K., Nishibori M., Fujita T., Kasai H., Nishibori E., Chiba N., Seong G., Tomai T. and Adschiri T. Fusion Growth and Extraordinary Distortion of Ultrasmall Metal Oxide Nanoparticles *Journal of the American Chemical Society* 146, 16324-31 (2024).

NASICON solid electrolytes:

Relative density links strength and conductivity

A viewpoint uncovers a unifying strategy to enhance performance and durability in sodium-ion batteries

28 July 2025

Corresponding Researcher

Eric Jianfeng Cheng

Associate Professor



website >>>



— Article highlight

Sodium superionic conductors with NASICON-type structures—such as $\text{Na}_{1+x}\text{Zr}_2\text{Si}_x\text{P}_{3-x}\text{O}_{12}$ (NZSP)—are promising solid electrolytes for solid-state sodium batteries due to their high ionic conductivity, wide electrochemical window, and compatibility with sodium metal. Yet, translating these materials into practical applications requires balancing two fundamentally different properties: ionic conductivity, which depends on atomic-scale ion mobility, and mechanical strength, which is shaped by microstructural features like porosity and grain bonding.

However, because these properties arise from distinct mechanisms, their relationship is not straightforward. In fact, past efforts to improve one often compromised the other. As a result, establishing a general, statistically robust correlation between the two properties has remained a key challenge in the design of high-performance solid electrolytes.

In a 2024 viewpoint article, researchers at Tohoku University's Advanced Institute for Materials Research (AIMR) conducted a comprehensive meta-analysis of experimental data from the literature¹. The team focused on sintered polycrystalline NZSP, a widely studied NASICON solid electrolyte, and applied statistical methods to evaluate the relationship between its mechanical properties—particularly hardness—and ionic conductivity across various compositions.

“We took a novel approach by emphasizing the role of relative density—a measure of how dense a material is compared to its theoretical maximum,” explains Eric Jianfeng Cheng, first author of the article. “We found that this microstructural parameter consistently influences both hardness and ionic conductivity across the dataset, more reliably than factors like doping or grain size.”

One key finding of the article is that hardness, a readily measurable mechanical property, can serve as a reliable predictor of ionic conductivity in oxide solid electrolytes. This insight provides researchers with a practical and efficient screening metric, and points to relative density optimization—through techniques like spark plasma sintering or sintering aid selection—as a unified strategy to improve both durability and performance in next-generation sodium-ion batteries.

“Following these results, one of our future directions is to further investigate the interplay between mechanical and electrochemical properties in solid electrolytes,” says Cheng. “This includes exploring potential approaches such as atomic-scale analysis to deepen the understanding of the underlying correlations.”

— A personal insight from Dr. Eric Jianfeng Cheng

What part of this research gave you the greatest sense of accomplishment, and why?

The most rewarding part of this work was proposing—and then finding preliminary evidence for—a positive correlation between hardness and ionic conductivity in NASICON-type solid electrolytes. These two properties are typically treated as separate, even competing, so it was exciting to uncover a potential link

between them. Because this connection wasn't obvious at first, seeing it emerge through careful data analysis gave me a real sense of accomplishment. It suggests a path forward that could help guide future materials research in a more integrated way.

Highlight Article

1. Cheng E.J., Yang T., Liu Y., Chai L., Garcia-Mendez R., Kazyak E., Fu Z., Luo G., Chen F., Inada R., Badilita V., Duan H., Wang Z., Qin J., Li H., Orimo S. and Kato H. Correlation between mechanical properties and ionic conductivity of polycrystalline sodium superionic conductors: A relative density-dominant relationship *Materials Today Energy* 44, 101644 (2024).

Spintronic devices:

Switching of magnetic memory bits with magnons

Crystal symmetry, spin canting, and magnon torques drive field-free out-of-plane magnetization switching in layered spintronic devices

25 August 2025

Corresponding Researcher

Mehrdad Elyasi

Assistant Professor



website >>>



— Article highlight

Magnetization switching remains one of the central applications of spintronic devices.

“Useful devices, such as magnetic memory or logic circuits, require the ability to switch individual magnetic bits without disturbing neighboring ones,” explains Mehrdad Elyasi, a member of AIMR. “This means technologically relevant solutions must not require global magnetic fields or high-power current inputs to achieve localized deterministic switching.”

To this end, a promising approach uses quasiparticles called magnons—wave-like magnetic disturbances that, in principle, can be confined, guided, or even generated locally, particularly using patterned nanostructures or pulsed excitations.

However, recent work on materials with perpendicular magnetic anisotropy (PMA)—ideal for high-density memory—showed that magnons could only switch magnetization reliably in the presence of an external magnetic field.

To overcome this, researchers needed a way to produce a controlled, out-of-plane spin-polarized magnon currents strong enough to deterministically switch PMA materials—without relying on external fields.

In a 2024 article, Elyasi and co-workers addressed this challenge by exploiting the crystal symmetry and spin canting angle of WTe_2 to generate the desired magnon torque in a $WTe_2/NiO/CoFeB$ heterostructure¹. The team used the low symmetry of WTe_2 to produce spin-polarized electrons with both in-plane and out-of-

plane components, which were injected into the adjacent NiO layer. The NiO antiferromagnetic insulator then converted the spin current into magnon currents, preserving their original polarization direction—a slight out-of-plane canting angle of approximately 8.5° .

“The out-of-plane tilt, preserved by the optimal NiO thickness of 25 nanometers, is the crucial feature that provides the anti-damping magnon torque required for deterministic switching of the CoFeB ferromagnet’s perpendicular magnetization without any external magnetic field,” says Elyasi. “Moreover, by acting as an insulating spacer, the NiO layer helps address thermal stability concerns by reducing the impact of Joule heating on the CoFeB layer—a key challenge as magnetic elements scale down.”

In addition to demonstrating field-free switching of perpendicular magnetization at room temperature with a critical current density as low as 4×10^6 A/cm², the authors further showed that introducing a PtTe₂ layer enhances in-plane conductivity while preserving the out-of-plane spin canting—reducing power consumption by a factor of 190 compared to earlier systems.

These results suggest that exploiting crystal symmetry and spin canting accompanied by magnon transport enables robust, energy-efficient switching. The work provides a blueprint for future low-power spintronic memory devices based on magnon currents.

As a next step, the researchers plan to investigate how nonlinear interactions between magnons may further contribute to spin angular momentum transfer from NiO to the magnetic layer.

— A personal insight from Dr. Mehrdad Elyasi

Do you have any reflections on this project and how it shaped you as a research scientist?

This project was especially meaningful for me as it marked the renewal of my scientific collaboration with Prof. Hyunsoo Yang, my former PhD advisor at the National University of Singapore (NUS). After several years, I visited his lab to present my recent works in magnonics, which led to fruitful discussions with Prof. Yang and the two equally contributing first authors,

Dr. Fei Wang and Dr. Guoyi Shi. From there, we collaborated closely—combining theory and experiment—to develop and publish this work. I’m proud of how it tackles a real technological challenge with both conceptual clarity and rigorous control, appealing to both physics and engineering communities.

Highlight Article

1. Wang F., Shi G., Yang D., Tan H.R., Zhang C., Lei J., Pu Y., Yang S., Soumyanarayanan A., Elyasi M. and Yang H. Deterministic switching of perpendicular magnetization by out-of-plane anti-damping magnon torques *Nature Nanotechnology* 19, 1478-1484 (2024).

Celestial mechanics: New analytical model reveals true cause of orbit bifurcations near Lagrange points

AIMR researchers unify the dynamics of Lissajous, halo, and quasi-halo orbits in the restricted three-body problem

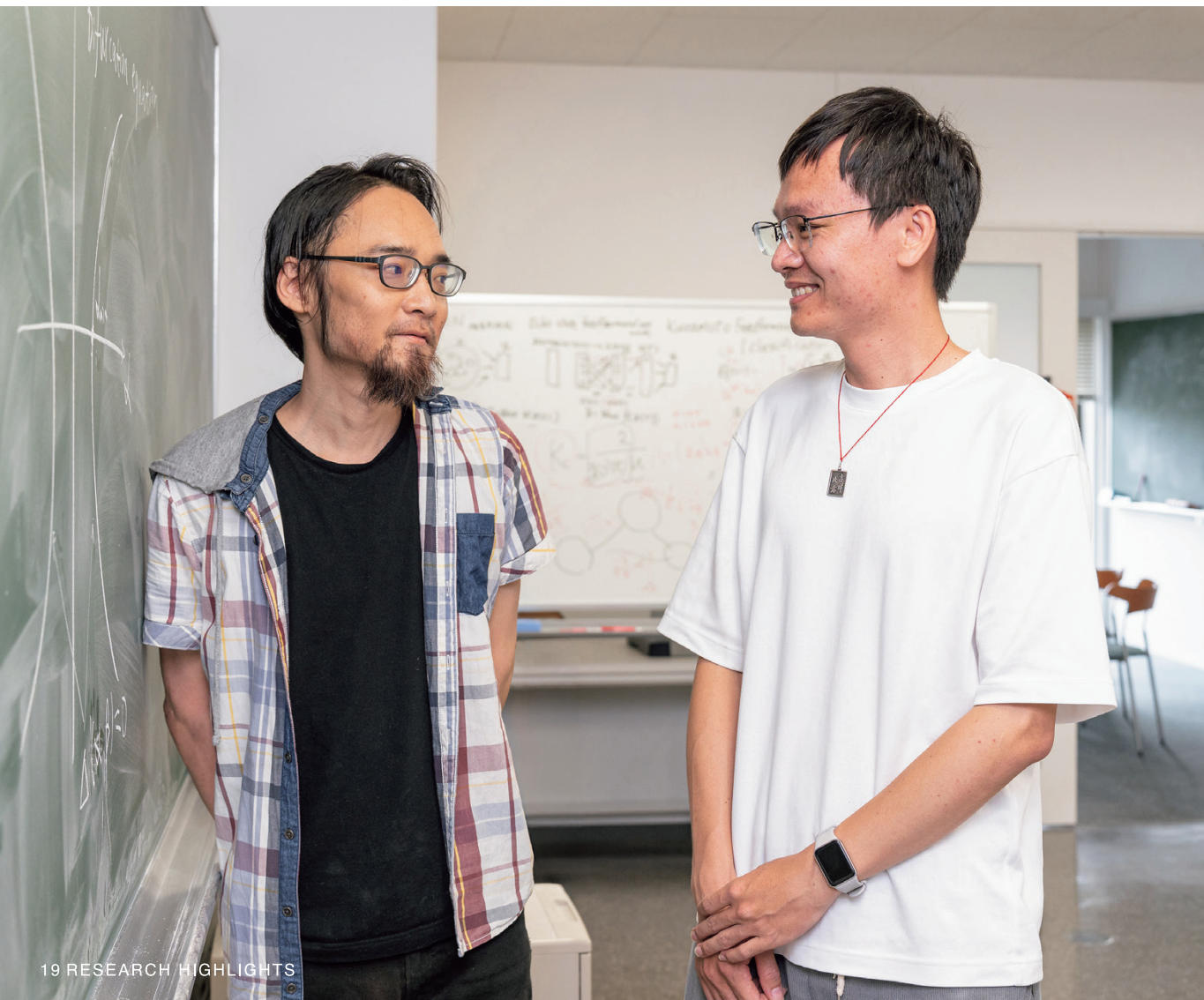
22 September 2025

Corresponding Researchers

Hayato Chiba **Mingpei Lin**

Principal Investigator

Assistant Professor



— Article highlight

Advanced space travel relies on a fundamental understanding of the restricted three-body problem (RTBP), in which one of the three bodies—typically a spacecraft—is so small that its gravity doesn't affect the other two, such as a planet and its moon.

"In RTBP systems, Lagrange points between the two celestial bodies provide specific locations around which a spacecraft can orbit," explains Mingpei Lin, a member of an AIMR research team. "The ability to model how complex orbits—such as halo, and quasi-halo orbits—emerge around the unstable collinear Lagrange points enables better trajectory design using these points."

However, a persistent challenge has been the lack of a unified analytical method for describing all types of Lagrange point orbits. Numerical simulations can model individual trajectories but are computationally intensive and system-specific. Existing analytical methods offer only fragmented solutions—handling Lissajous or halo orbits separately, and failing to capture quasi-halo orbits altogether.

In a 2024 article, Lin and Chiba developed a unified analytical framework to describe the center manifolds of collinear Lagrange points in the RTBP¹. Their method introduces a coupling mechanism that explains how quasi-halo orbits bifurcate from Lissajous orbits—without requiring frequency resonance.

"Previous analytical models treated frequency resonance as the main mechanism behind the emergence

of complex orbits," says Lin. "But this approach couldn't account for the bifurcation of quasi-halo orbits from Lissajous orbits, and numerical observations also pointed to a different behavior. Based on this, we proposed that nonlinear coupling—not resonance—is the true cause of orbit bifurcations, a dynamic no existing model had captured adequately."

The novelty of the team's approach lies in introducing a coupling coefficient, η , and a bifurcation equation, $\Delta = 0$, into the RTBP equations. This modification preserves the nonlinear coupling between in-plane and out-of-plane motions, allowing bifurcations to emerge naturally—and without relying on resonance conditions.

The result is a high-order series solution that analytically describes Lissajous, halo, and quasi-halo orbits within the same formalism: when $\eta = 0$, the solution yields Lissajous orbits; when $\eta \neq 0$, it captures quasi-halo orbits, with halo orbits appearing as special cases.

"This breakthrough transforms the understanding of orbital dynamics near Lagrange points," concludes Lin. "Our work enables precise analytical modeling of all known center manifold orbit types—greatly benefiting space mission design and bifurcation theory alike."

The team is now extending this coupling-induced bifurcation framework to other dynamical systems, including modeling symmetry-breaking phenomena such as the evolution of right-handedness in humans.

— A personal insight from Dr. Mingpei Lin

What part of this research gave you the greatest sense of accomplishment, and why?

The challenge of explaining why bifurcated two-dimensional tori resist semi-analytical solutions has intrigued me since the early days of my PhD, but other projects delayed a focused investigation. At Chiba Laboratory in AIMR, I finally had the time and space to explore it deeply. After many failed attempts using conventional approaches, we began questioning

the half-century-old resonance mechanism. This shift led to a key insight: coupling interactions—not resonance—drive this local bifurcation. Developing the coupling-induced bifurcation mechanism and explaining halo/quasi-halo orbits resolved a seven-year puzzle for me and boosted my confidence to explore the unknown.

Highlight Article

1. Lin M. and Chiba H. Bifurcation mechanism of quasi-halo orbit from Lissajous orbit *Journal of Guidance, Control, and Dynamics* 48, 71-83 (2024).

Quantum metric: Flexible control of electronic-state geometry in real materials

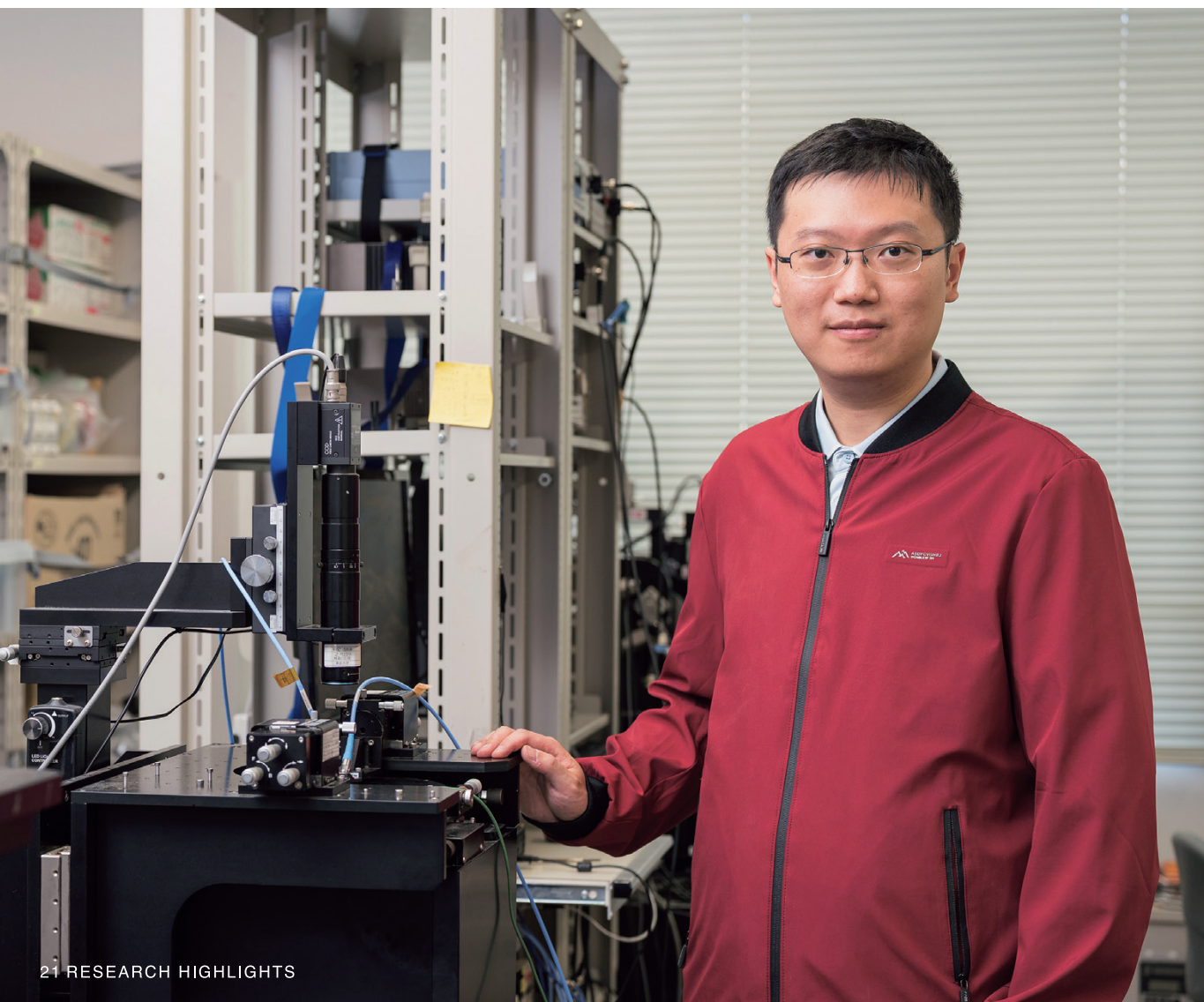
Researchers demonstrate manipulation of quantum metric in Mn₃Sn/Pt heterostructures under ambient conditions

27 October 2025

Corresponding Researcher

Jiahao Han

Associate Professor



website >>>



— Article highlight

Scientists have long sought to understand the quantum metric (QM)—a fundamental quantity that measures how rapidly neighboring electronic states in a solid change across momentum space. Predicted to drive exotic nonlinear and topological responses, QM has remained experimentally unexplored because this hidden wavefunction property is thought to be fragile under ambient conditions.

“Previous observations hinted at QM effects, but only under conditions that required van der Waals magnets, liquid-helium cooling, and multi-tesla fields,” says Jiahao Han, a member of an AIMR research team.

In a 2024 article, Han *et al.* showed that the QM can not only be detected but also tuned under ambient conditions¹. They achieved this by engineering a heterostructure of the chiral antiferromagnet Mn₃Sn capped with Pt, where interfacial spin textures offer a means to control the underlying QM.

“The novelty of this work was that by capping Mn₃Sn with a thin Pt layer, we engineered interfacial spin textures that break both inversion and time-reversal symmetries,” explains Han. “This symmetry breaking is what allows the QM contributions to stand out clearly in electrical measurements.”

By tracking the nonlinear Hall response in their heterostructure, the team showed that QM manifests as a time-reversal-odd second-order Hall effect. Remarkably, this signal remained robust across a wide temperature range—from cryogenic levels up to well above room temperature—and could be reversibly switched with small external magnetic fields, confirming the ability to flexibly control the QM.

“The significance of this result is that it establishes a practical route to harnessing quantum geometry in real materials,” says Han. “Being able to control QM under ambient conditions opens new opportunities for topological electronics, from low-power memory and logic elements to sensors and rectifiers that exploit the geometry of electronic states rather than just their charge or spin.”

A future direction will use this approach to explore unconventional superconductivity in flat-band and topological systems, as well as other facets of quantum geometry for transport phenomena and device applications.

— A personal insight from Dr. Jiahao Han

What idea or moment in this project gave you the deepest sense of accomplishment, and did anything about the results surprise you?

For me, the greatest accomplishment was conceiving the idea of using the Mn₃Sn interface to engineer a spin texture that simultaneously breaks inversion and time-reversal symmetries. This approach was crucial to making the quantum metric visible in a second-order Hall effect, and it drew on insights from materials science, spintronics, and geometric physics

in a way that felt very innovative. What impressed me most was how effectively the experiment realized this conception. It wasn't so much surprising as deeply satisfying to see our thorough understanding of chiral antiferromagnets translate so directly into successful experimental outcomes.

Highlight Article

1. Han J., Uchimura T., Araki Y., Yoon J.-Y., Takeuchi Y., Yamane Y., Kanai S., Ieda J., Ohno H. and Fukami S. Room-temperature flexible manipulation of the quantum-metric structure in a topological chiral antiferromagnet *Nature Physics* 20, 1110-1117 (2024).

Carbon-material analysis:

Ultra-high-temperature TPD identifies hidden nitrogen environments

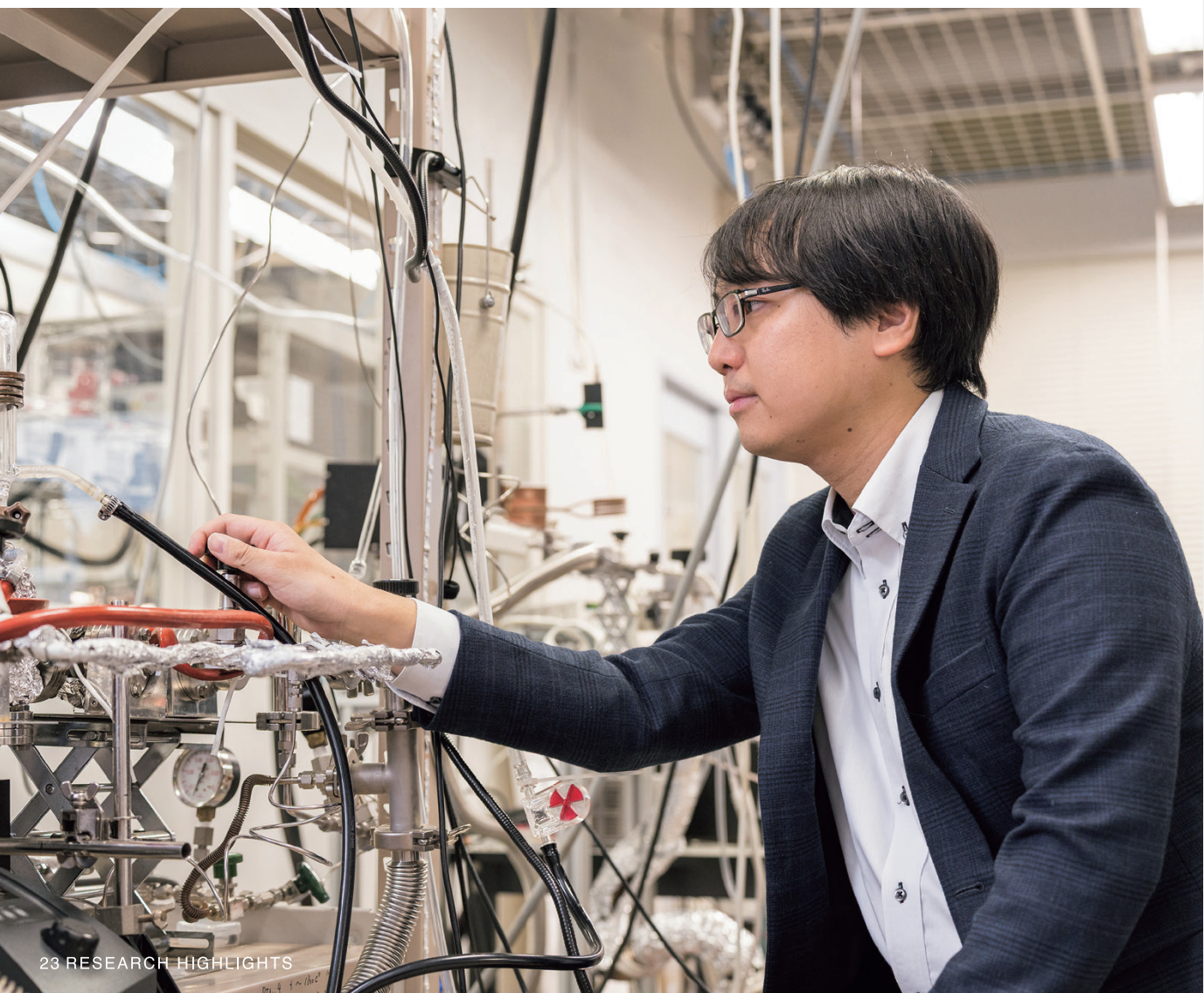
Novel analytical approach reveals nitrogen bonding states previously inaccessible to conventional techniques

25 November 2025

Corresponding Researcher

Takeharu Yoshii

Associate Professor



website >>>



— Article highlight

Scientists have long sought to understand how nitrogen atoms (N) are incorporated into carbon materials—such as graphene, graphite, and nanodiamonds—because the modes of N-doping strongly influence their catalytic and electronic properties. Developing a reliable method for both qualitative and quantitative characterization of nitrogen bonding states is essential for improving materials used in batteries, fuel cells, and sensors.

However, common probing techniques such as X-ray photoelectron spectroscopy (XPS) and CHN elemental analysis provide only surface-level or bulk composition data at limited sensitivity. They often fail to distinguish between different nitrogen environments—pyrrolic, pyridinic, and graphitic—especially when the N content is at trace levels below 1,000 ppm.

The lack of accurate, high-resolution methods for nitrogen speciation has hindered the rational design of N-doped materials and the resolution of long-standing industrial problems related to trace nitrogen in carbon.

In a 2024 article, Takeharu Yoshii, Hiroto Nishihara, and co-workers from the Advanced Institute for Materials Research (AIMR) at Tohoku University addressed this challenge with a novel analytical approach¹. Using vacuum temperature-programmed desorption (TPD) capable of heating carbon samples to 2,100 °C, the team achieved complete desorption of N species from designed carbon structures and measured the evolved gases—NH₃, HCN, and N₂—with unprecedented sensitivity.

Unlike conventional surface-sensitive methods, this destructive approach enables full quantitative analysis of nitrogen within the bulk.

“Our key innovation is combining an ultra-high-temperature vacuum TPD system with mass spectrometric (MS) detection and a purpose-designed N-doped carbon material (N-CMS) composed of rarely stacked, curved graphene sheets,” explains Yoshii. “This integration enabled complete desorption of nitrogen species and a direct correlation between the evolved gases and specific nitrogen environments.”

Using complementary density-functional theory modeling to analyze the MS results, the team showed that in N-CMS, pyrrolic-N releases NH₃ and HCN, pyridinic-N produces HCN and N₂, and graphitic-N yields only N₂ at higher temperatures.

The technique also provided precise qualitative and quantitative determination of nitrogen in diverse carbon materials, including industrial coke, where XPS failed to detect buried nitrogen atoms.

“When we applied the technique to nitrogen-containing coke, we detected only N₂ desorption above 1,200 degrees Celsius,” says Yoshii. “This indicated that nearly all the nitrogen existed in stable graphitic environments, which conventional XPS could not capture because much of it was buried deep within the carbon structure.”

By achieving two orders of magnitude higher sensitivity than previous methods, this work establishes ultra-high-temperature TPD as a transformative and complementary tool for understanding and controlling nitrogen chemistry in carbon materials, with broad implications for catalysis, energy storage, and materials manufacturing.

— A personal insight from Dr. Takeharu Yoshii

What part of this project gave you the greatest sense of accomplishment, and why?

For me, the biggest sense of accomplishment came when we finally proved that nitrogen dopants in carbon materials can be identified using a destructive analytical method. Reaching 2,100 °C to achieve complete desorption and quantification of all nitrogen species was something no one had done before.

Getting there wasn't easy—we had to design hardware that could survive ultra-high temperatures, calibrate toxic HCN gas, and separate CO and N₂ signals that share the same mass. After years of trial and error, seeing clear evidence of each nitrogen bonding state was an incredibly satisfying moment.

Highlight Article

1. Yoshii T., Nishikawa G., Kumar Prasad V., Shimizu S., Kawaguchi R., Tang R., Chida K., Sato N., Sakamoto R., Takatani K., Moreno-Rodriguez D., Škorňa P., Scholtzová E., Karoly Szilagyi R. and Nishihara H. Quantitative and qualitative analysis of nitrogen species in carbon at the ppm level *Chem* 10, 2450-63 (2024).

Solid-state ionics: Review article reveals structural blueprint for superionic conductors

Framework connectivity unlocks secrets of fast ion transport in next-generation battery materials

22 December 2025

Corresponding Researchers

Shin-ichi Orimo

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website >>>



— Article highlight

A central question in solid-state ionics is what structural and chemical factors enable certain solids to conduct ions as efficiently as liquids. Understanding this phenomenon is essential for developing new all-solid-state batteries that can surpass conventional lithium-ion systems in both energy density and operational safety.

However, despite decades of progress, researchers have struggled to identify consistent design principles for fast ion conductors.

“Ionic conductivity can vary widely even among materials with similar structures,” explains Kartik Sau, a member of the AIMR research team. “Subtle differences in crystal framework, bottleneck geometry, and ion–ion interactions can drastically alter ion mobility. This complexity has made it difficult to move beyond empirical discovery toward predictive, theory-driven design.”

In a 2024 review article, the team led by Kartik Sau and Shin-ichi Orimo examined recent advances across multiple classes of solid fast-ion conductors—layered oxides, polyhedral frameworks, and cluster-anion materials¹. Synthesizing experimental observations and theoretical insights, their review sought to clarify the fundamental relationships between structure and ion transport.

What sets this review apart is its structural perspective. Rather than classifying materials by their chemical composition, the authors organized them according to the connectivity of their anion frameworks—the structural scaffolds that define ion migration pathways.

This framework-centered view revealed universal design principles, including three-dimensional interstitial networks, polarizable anion lattices, and cooperative ion motion, that underpin fast ionic conduction across diverse material families.

“Our structural perspective allowed us to identify broader trends,” says Sau. “For instance, materials with flexible, polarizable frameworks—particularly halide- and hydride-based conductors—can achieve room-temperature ionic conductivities of 25–70 mS cm⁻¹ and activation energies as low as 0.1–0.3 eV. Examples such as Li_{9.54}Si_{1.74}P_{1.44}S_{11.7}Cl_{0.3} (25 mS cm⁻¹) and Na₂(CB₉H₁₀)(CB₁₁H₁₂) (70 mS cm⁻¹) rival the performance of liquid electrolytes.”

By consolidating structure-property relationships across diverse systems, this review provides a clear blueprint for designing next-generation solid electrolytes. Its framework-centered perspective equips researchers to engineer materials with predictable, high ionic conductivities—accelerating progress toward safer and more powerful all-solid-state batteries.

Building on these insights, the team is now focusing on anion rotation mechanisms, material alloying strategies, and machine learning approaches to accelerate the discovery of new fast-ion conductors that balance high performance with the electrochemical stability and safety required for commercial applications.

— A personal insight from Dr. Kartik Sau

What part of this research gave you the greatest sense of accomplishment, and what potential societal impact do you foresee?

The most satisfying aspect was transforming decades of scattered research into a clear, usable framework for materials design. After more than a decade working in fast-ion conduction, I recognized several underappreciated directions: the role of rotating polyhedral anions, distinct design guidelines for lithium versus sodium systems, and principles for multivalent

ions like Mg²⁺ and Ca²⁺. This review provided a platform to turn these insights into simple design rules. Looking ahead, I envision these guidelines accelerating safer, higher-capacity batteries for electric vehicles and grid-scale renewable storage, with machine learning opening new chemical spaces and opportunities in barocaloric cooling and advanced sensing applications.

Highlight Article

1. Sau K., Takagi S., Ikeshoji T., Kisu K., Sato R., Campos dos Santos E., Li H., Mohtadi R. and Orimo S. Unlocking the secrets of ideal fast ion conductors for all-solid-state batteries *Communications Materials* 5, 122 (2024).

Materials chemistry: Uncovering the low-temperature oxygen storage and release mechanism of Mn–CeO₂ nanoparticles

Precise continuous-flow synthesis reveals how Mn valence and local structure control lattice oxygen storage and release in ultrasmall ceria-based nanoparticles

26 January 2026

Corresponding Researcher

Chunli Han

Specially Appointed Assistant Professor

website »»



— Article highlight

The search for better oxygen carriers has long centered on one key question: how can we design metal oxides that can reversibly store and release lattice oxygen efficiently at lower temperatures? This reversible behavior underpins clean-energy technologies such as fuel conversion, CO₂ capture, and chemical looping for hydrogen production, where reaction feasibility and efficiency depend directly on a material's oxygen storage and release capacity (OSC).

Among these candidate materials, doped ceria (CeO₂) has been a particularly promising system for achieving high and tunable oxygen mobility.

However, researchers struggled to connect OSC property with the detailed local structure and chemical state of doped ceria nanoparticles. Traditional synthesis methods could not precisely control dopant inclusion state, dispersion, or valence, leading to inconsistent samples and obscuring the mechanisms behind oxygen storage and release at different temperatures.

In a 2025 article¹, an AIMR research team led by Chunli Han, Akira Yoko, and Tadafumi Adschiri addressed this challenge through a continuous-flow hydrothermal synthesis method capable of producing ultrasmall Mn-doped CeO₂ nanoparticles with tightly controlled structural and chemical features. This approach enabled rapid heating, mixing, and quenching—on timescales of milliseconds to seconds—allowing the authors to tune Mn inclusion state (in or out of the CeO₂ lattice) and chemical state with unusual precision.

A key innovation was the precise thermodynamic and kinetic co-control of the dopant-host atom assembly and distribution based on the swift start-up flow hydrothermal synthesis system.

“By controlling the residence time and relative precipitation rates of the Mn and Ce precursors, we could stabilize CeO₂ nanoparticles smaller than five nanometers while capturing diverse Mn environments,” explains Han. “This includes lattice-substituted Mn atoms, surface Mn species, and phase-segregated MnO_x—local structures that conventional batch syntheses cannot reliably produce.”

The resulting Mn–CeO₂ nanoparticles exhibited a fourfold increase in low-temperature (< 300 °C) OSC compared with particles made by batch methods. The work also showed that low-temperature OSC is mainly enhanced by Mn²⁺ substitution in the CeO₂ lattice and surface Mn species, whereas high-temperature (≥ 300 °C) OSC correlates with overall Mn and Ce³⁺ concentrations, regardless of how Mn is incorporated into the CeO₂.

These findings demonstrate that precise control over dopant valence and local structure is essential for uncovering the mechanisms behind oxygen storage and release and for designing higher-performing low-temperature oxygen carriers. More broadly, the study highlights continuous-flow synthesis as a controllable and scalable route to functional nanoparticles and underscores the importance of precise materials synthesis for advancing both practical applications and fundamental understanding.

— A personal insight from Dr. Chunli Han

What aspect of this work do you believe will have the greatest impact on future research and real-world applications?

What stood out most to me in this project was realizing how much control we could gain by shifting from traditional thermodynamic thinking to process-based kinetic control at the millisecond scale. Instead of focusing only on nanoparticle size and shape, we began controlling the atom distribution, ordering, coordination, and chemical state by precisely controlling

the reaction field—mixing, heat and mass transfer, and kinetic pathways. This opens the door to uncovering many of the “black boxes” in batch synthesis. And because continuous-flow methods are reproducible and scalable, I believe this approach will help bridge the gap between laboratory discoveries and real-world applications much more quickly.

Highlight Article

1. Han C., Yoko A., Taufik A., Ohara S., Nishibori M., Ninomiya K., Kiuchi H., Harada Y., and Adschiri T. High oxygen storage capacity of ultrasmall Mn-doped CeO₂ nanoparticles via enhanced local distortion and Mn(II) lattice substitution *Chemistry of Materials* 37, 1205-14 (2025).



(6,5) Carbon nanotubes: Ultrahigh-purity synthesis achieved through trimetallic catalyst innovation

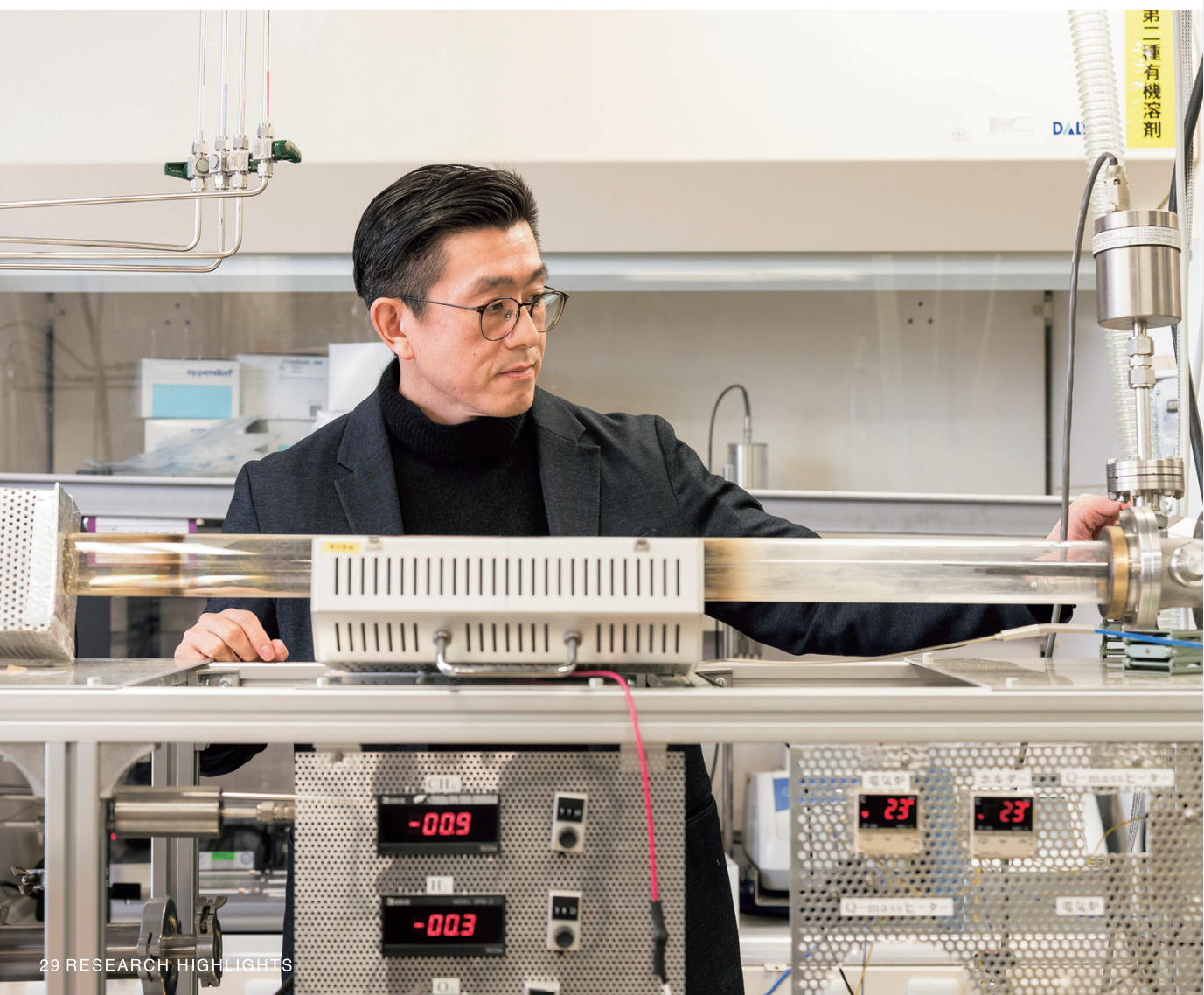
NiSnFe catalyst enables 95.8% purity synthesis
of semiconductor carbon nanotubes with ideal bandgap properties

24 February 2026

Corresponding Researcher

Toshiaki Kato

Principal Investigator



website >>>



— Article highlight

A central scientific question in carbon nanotube (CNT) research remains whether single-walled CNTs can be synthesized with direct control of chirality, particularly for small-diameter semiconducting species that are technologically useful. Achieving such control is essential because a nanotube's chirality determines its electronic band gap, optical response, and device performance.

However, current growth methods produce broad mixtures of chiralities, and even syntheses termed “selective” rarely exceed moderate purity, typically in the 50–80 % range. While direct synthesis with over 90 % purity has been demonstrated for a small number of chiralities—most notably (14,4)- and (12,6)-CNTs—important targets such as (6,5)-CNTs have remained well out of reach.

In a 2024 article, an AIMR research team led by Toshiaki Kato reported a breakthrough approach that addresses this limitation by redesigning the catalyst itself¹. The team demonstrated that a carefully engineered trimetallic catalyst can precisely control the energetics of nanotube growth, enabling near-single-chirality synthesis that was previously inaccessible.

“The novelty of this work lies in the use of a NiSnFe trimetallic catalyst in which partial formation of Ni₃Sn intermetallic crystals occurs within nanoscale catalyst particles,” explains Kato. “This specific phase selectively lowers the activation energy for the growth of (6,5)-CNTs during plasma-enhanced chemical vapor deposition, while suppressing competing chiralities.”

Using this approach, the authors achieved an ultrahigh-purity synthesis of (6,5)-CNTs, reaching approximately 95.8% purity as confirmed by photoluminescence, UV–vis–NIR spectroscopy, and Raman analysis. They also observed the direct formation of chirality-pure (6,5)-CNT bundles and measured photoluminescence lifetimes more than 20 times longer than those of isolated tubes.

“Previous mono- and bimetallic catalysts can bias nanotube growth, but their ability to discriminate between closely competing chiralities is fundamentally limited,” says Kato. “We discovered that a trimetallic system can stabilize a specific intermetallic phase within the catalyst nanoparticles, which provides an additional level of thermodynamic control and—in this case—favors the nucleation of (6,5)-CNTs.”

The results from this work demonstrated that intermetallic catalyst phases can be used to engineer chirality selection at the atomic level, providing a general strategy for single-chirality nanotube growth. Beyond synthesis, the formation of chirality-pure bundles with enhanced excitonic properties opens new opportunities for optoelectronic and quantum photonic applications.

A future direction involves extending this multi-element catalyst approach to synthesize other single-chirality nanotubes on demand for semiconductor and quantum devices.

— A personal insight from Dr. Toshiaki Kato

Looking back on this project, what stands out most about the discovery process and its significance?

The most memorable aspect was the discovery itself — a master's student found the breakthrough catalyst somewhat by chance while systematically searching through catalyst combinations. What made this particularly satisfying was our ability to explain why it worked through detailed structural analysis, proposing a growth model that validated the

experimental results. Catalysts with three or more elements had never been explored for CNT synthesis—it was outside conventional thinking. By challenging previous assumptions, we opened an entirely new research direction. Proving that our intuition was correct has been deeply encouraging and provides a design principle for future catalyst development.

Highlight Article

1. Shiina S., Murohashi T., Ishibashi K., He X., Koretsune T., Liu Z., Terashima W., Kato Y.K., Inoue K., Saito M., Ikuhara Y. and Kato T. Synthesis of ultrahigh-purity (6,5) carbon nanotubes using a trimetallic catalyst *ACS Nano* 18, 23979-90 (2024).



Neural networks: Directional wiring shapes biologically relevant activity patterns in engineered networks

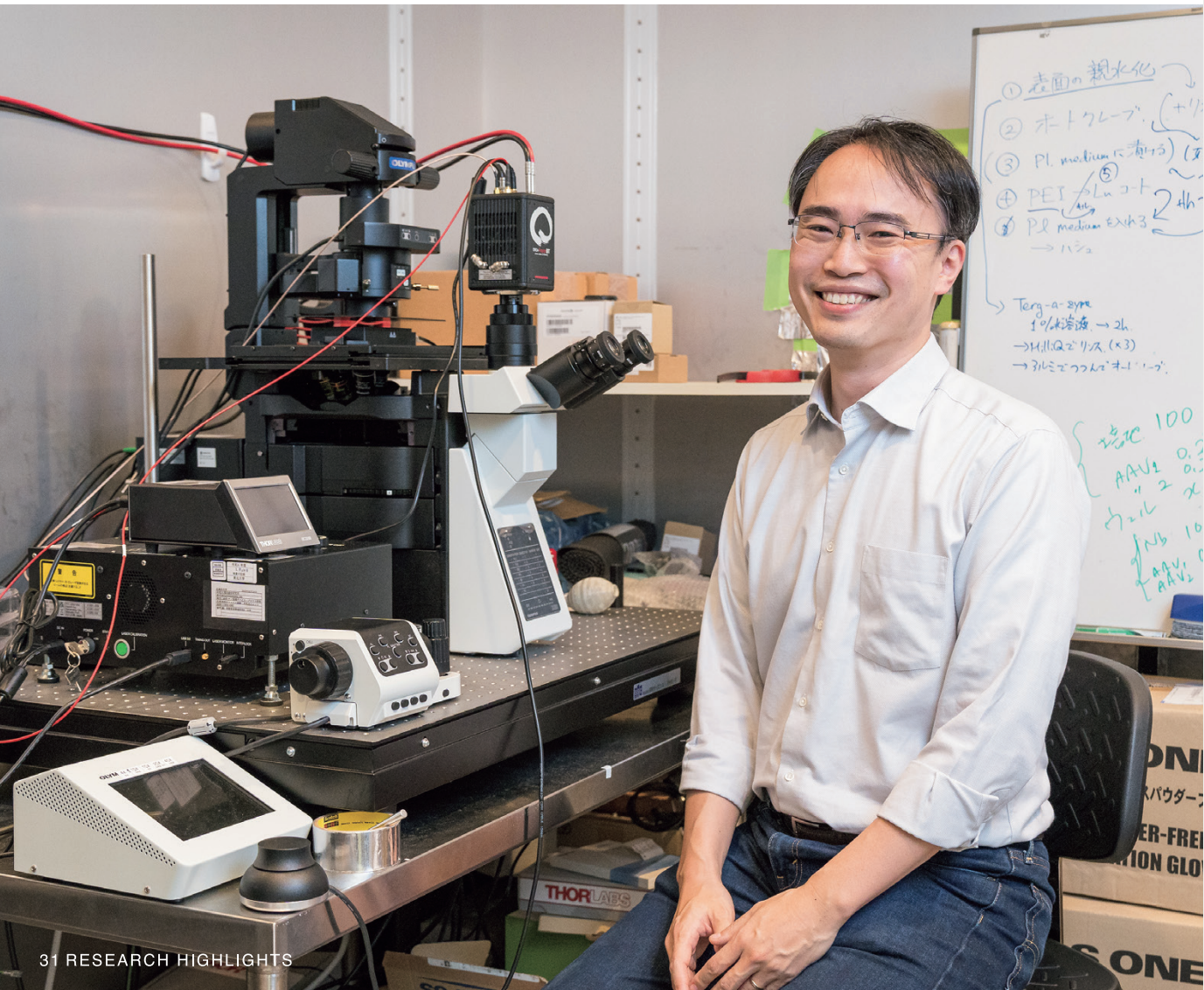
Microfluidic brain-on-a-chip platform reveals how hierarchical modularity and axon-to-dendrite connectivity regulate the balance between integration and segregation

23 March 2026

Corresponding Researcher

Hideaki Yamamoto

Associate Professor



— Article highlight

The brain is not a random collection of neurons. Across species, evolution has preserved key hierarchical architectural features, including modular organization, characterized by patches of densely clustered neurons, and directional wiring shaped by axon-to-dendrite signaling. How these structural features shape patterns of activity across neural networks remains an open question.

To this end, a standing question in neuroscience has been how these structural features shape collective neural dynamics. Specifically, how modular organization and directional connectivity influence the balance between globally synchronized activity and locally specialized, independent patterns across a network.

However, answering this question has been technically challenging.

“In conventional *in vitro* neuronal cultures, neurons tend to form largely homogeneous and highly reciprocal connections, often leading to excessive network-wide synchrony that masks the distinct roles of modular structure and directional connectivity,” says Hideaki Yamamoto, a researcher at AIMR. “When activity becomes globally synchronized, it is difficult to determine whether the dynamics reflect modular architecture or simply strong overall coupling.”

In a 2025 article, Yamamoto and co-workers addressed this challenge by integrating *in vitro* experiments with computational and mathematical modeling¹.

“Experimentally, we used microfabricated devices to guide axonal growth and construct hierarchically modular networks with defined directional coupling between modules,” explains Yamamoto. “In parallel,

we used spiking neural network (SNN) simulations and state-transition mathematical models to provide a framework for predicting how such architectures would regulate global synchrony. This combined experimental–theoretical approach enabled us to isolate the effects of network structure on collective neural dynamics.”

The key innovation of this work was the use of microfluidic devices containing asymmetrically tapered microchannels that bias axonal growth in a preferred direction. This geometry reinforces axon-to-dendrite connectivity between modules, favoring feedforward signaling across the network—an architecture not attainable in conventional cultures.

The *in vitro* experiments demonstrated that, rather than the uniform network-wide activation observed in conventional cultures, activity in the engineered networks propagated directionally between modules, producing more spatially segregated dynamics. Moreover, the SNN simulations and state-transition models not only reproduced these experimental observations but also enabled analytical predictions of how network topology shapes dynamics.

“Our work shows that the brain’s hierarchical and directional architecture isn’t arbitrary—these features actively regulate the balance between integrated and segregated activity patterns that makes complex behavior possible,” explains Yamamoto. “The new *in vitro* platform now enables us to apply these principles both in pharmacological research for drug discovery and as a foundation for brain-inspired biocomputing systems.”

— A personal insight from Dr. Hideaki Yamamoto

What aspect of this research gave you the greatest sense of accomplishment, and what surprised you most during the project?

My greatest sense of accomplishment came from demonstrating that directional connectivity and modular structure successfully suppress excessive synchrony in cultured neuronal networks—mirroring their role in the brain. This showed that brain-like architectures produce biologically grounded dynamics even *in vitro*. What surprised me most was discovering the power of integrating multiple disciplines—biology,

physics, engineering, and mathematics. By bridging experiment and theory, we extracted universal principles governing network dynamics. Combining *in vitro* experiments, computational spiking neural network models, and mathematical state-transition models allowed us not just to observe phenomena but to understand and predict the underlying mechanisms analytically.

Highlight Article

1. Monma N., Yamamoto H., Fujiwara N., Murota H., Moriya S., Hirano-Iwata A. and Sato S. Directional intermodular coupling enriches functional complexity in biological neuronal networks *Neural Networks* 184 106967 (2025).

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