ISSN 1342-0321 IAREFM

ICR ANNUAL REPORT

2023

Volume 30

Institute for Chemical Research Kyoto University ICR

ICR ANNUAL REPORT 2023 (Volume 30) - ISSN 1342-0321 -

This Annual Report covers from 1 January to 31 December 2023

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Institute for Chemical Research (ICR), Kyoto University

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Request for Cooperation to the ICR's 100th Anniversary Fund

ICR has established a fund called "The ICR's 100th Anniversary Fund," which is a part of the Kyoto University Fund. Its aims are to hold the 100th anniversary event in 2026, to enhance the educational and research environments at ICR, and to promote social contribution activities. We ask for your kind understanding and cooperation.



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ICR ANNUAL REPORT 2023



Institute for Chemical Research Kyoto University

Volume 30





It is a great pleasure to publish the 30th volume of the Institute for Chemical Research (ICR) Annual Report. ICR was established as the first research institute of Kyoto University in 1926, with the founding philosophy "To Excel in the Investigation of Basic Principles of Chemistry and Their Applications." Since 1994, ICR Annual Report has been published annually to disseminate ICR's current activities worldwide. We currently have 120 faculty members, 200 graduate students, including 50 from abroad, and 60 researchers. These scientists are grouped into 30 laboratories divided into five research divisions-Synthetic Chemistry, Materials Chemistry, Biochemistry, Environmental Chemistry, and Multidisciplinary Chemistry-and three research centers-Advanced Research Center for Beam Science, International Research Center for Elements Science, and Bioinformatics Center. The laboratories are diversely affiliated with the graduate schools of science, engineering, agriculture, pharmaceutical sciences, medicine, and informatics.

The research of ICR encompasses a wide range of scientific disciplines, including physics, biology, and informatics as well as chemistry. ICR members conduct cuttingedge research not only in fields of their own specific disciplines but also in interdisciplinary and innovative fields. Some of outstanding research achievements in 2023 are as follows: 1) Unusual Nuclear Exchange within a Germanium-Containing Aromatic Ring that Results in Germanium Atom Transfer; 2)Synthesis of Tertiary Alkylphosphonate Oligonucleotides through Light-Driven Radical-Polar Crossover Reactions; 3) Location-Selective Immobilisation of Single-Atom Catalysts on the Surface or within the Interior of Ionic Nanocrystals Using Coordination Chemistry; 4) Magnetization Control of Zero-Field Intrinsic Superconducting Diode Effect; 5) Synergistic Surface Modification of Tin-Lead Perovskite Solar Cells; 6) Generation of Third-Harmonic Spin

Oscillation from Strong Spin Precession Induced by Terahertz Magnetic Near Fields; 7) Genomic Adaptation of Giant Viruses in Polar Oceans. Other distinctive achievements were presented also in the 123rd ICR Annual Symposium on December 1, 2023.

ICR collaborates with other research institutions on projects including MEXT Inter-University Collaborative Project "Integrated Consortium on Chemical Synthesis", MEXT Large-scale Scientific Research Project "Spintronics Research Network of Japan", and Research Unit for Realization of Sustainable Society in the Kyoto University Research Coordination Alliance. We have also been engaged in over 60 international collaborations with overseas universities and research institutions. In 2018, based on our strong global activity in chemistry-oriented fields, ICR was certified by MEXT as an International Joint Usage/Research Center. To encourage young researchers we have established several programs to support research and postgraduate education, including an in-house annual grant system, "ICR Grant for Promoting Integrated Research." These collaborative achievements underline our commitment to promoting ICR as a global research hub in chemistry-related fields.

The world around us is undergoing a wave of changes. The growing economy has exposed various global problems including climate change and social inequity. For a just and sustainable society, science and technology must become a credible beacon of light. ICR contributes to this goal by providing leadership and expertise in scientific research, fostering multidisciplinary, chemistry-related communities, and developing new and technologically significant innovations. We hope this Annual Report will serve to update you on the progress of our research activities and globalization. We appreciate your continued encouragement and support.

January 2024

ahash Soyamas

AOYAMA, Takashi Director

ICR News 2023

Recently Published in *Nature*! "Mirusviruses Link Herpesviruses to Giant Viruses"

MENG, Lingjie and Prof OGATA, Hiroyuki

On April 19th, our work was published in Nature. In this work, we discovered a novel group of large DNA viruses dubbed "*Mirusviricota*". Most of double stranded DNA viruses are classified into one of two realms: *Varidnaviria*, which includes giant viruses, and *Duplodnaviria*, which includes herpesviruses causing diseases in animals. These two realms have been considered evolutionarily unrelated. However, the newly discovered mirusviruses possess features of both realms. Genes of "informational module" for genome replication and gene expression were similar to those of *Varidnaviria*, while genes of "virion module" that encode structural proteins were similar to those of *Duplodnavira*. This mosaic feature

of mirusviruses suggests that herpesviruses evolved from tailed bacterial viruses via ancestral protist-infecting viruses, namely the ancestors of the modern day mirusviruses and herpesviruses. Furthermore, gene transfers of "informational genes" between the two realms probably played crucial roles in their evolution. Mirusviruses appear to be prevalent and abundant in the sea and likely infect a variety of protists. However, they were discovered by bioinformatics analyses of marine metagenomic data, and there are currently no cultured viruses from this group of viruses. This work was achieved by a collaboration with groups of scientists in France and Denmark.



10th Pacific Symposium on Radical Chemistry (PSRC-10)

PSRC-10 was held at Obaku Plaza, Uji Campus. Since its establishment in 2004, the PSRC has aimed to promote the development of organic radical chemistry in the world and mutual exchanges among researchers. A total of 186 researchers from 18 countries gathered for 55 oral research presentations (3 keynote lectures, 28 special invited lectures, and 24 invited lectures) and 91 poster presentations. Recent research results in a wide range of fields were presented, including reaction development using photo-redox catalysts, precise polymer synthesis, and theory of complex molecules in which multiple radicals interact with each other. The participants were able to interact with each other in a relaxed atmosphere. Twelve students and post-doctoral fellows were selected as poster award winners and presented with awards at the closing ceremony.

Through these activities, we believe that we have successfully achieved the original purpose of this conference, which was to further develop research in organic radical chemistry and to provide a forum for international exchange among the research community. We would like to express our deep appreciation for the cooperation and support not only of the conference participants, but also of all the people involved. Prof YAMAGO, Shigeru



New Collaboration Project Starts Memorandum of Understanding Signed between Sungkyunkwan University's Institute for Energy Science and Technology and ICR

Prof WAKAMIYA, Atsushi

On June 5, 2023, a delegation from Sungkyunkwan University (SKKU) led by Prof. Nam-Gyu Park, the director of SKKU's Institute of Energy Science and Technology, visited ICR. The purpose of the visit was to participate in the 1st Kyoto-SKKU Workshop, which was held in cooperation with Prof. Wakamiya's laboratory. During the workshop, a Memorandum of Understanding (MOU) was signed between the Institute of Energy Science and Technology, SKKU, and ICR, Kyoto University (Director, Prof. Takashi Aoyama) to encourage interdepartmental academic exchange. A collaborative project on perovskite solar cells was launched with the support of the International Collaborative Research Program of the Institute for Chemical Research (ICR), Kyoto University, and the Korean National Research Foundation (KNRF). This initiative led to the establishment of the SKKU-Kyoto University Perovskite International Research Collaboration Center (PIRCC) within the Institute of Energy Science and Technology at SKKU in Korea.



ICR Hosted Four Student Awardees from the Philippines

On the occasion of *Talent-Spot 2023 Manila* held in January 2023, ICR Travel Award was presented to 4 topperforming students out of 17 student candidates from the Philippines. In March 2023, the awardees, two of them were from University of the Philippines Diliman, and one each of the other two were from University of Santo Tomas and De La Salle University.

They were invited to participate in a week-long research training at the laboratory of their utmost interest at ICR, Kyoto University. At the conclusion of the training program, each of the awardees gave a short presentation of their research experience at ICR. Through the relaxed and open discussion, the students interacted with young researchers and faculty members of ICR to promote networking. One of the students, Matthew Denwell Herrera, will join an ICR laboratory as a MEXT scholar and pursue a Master's degree from Kyoto University.



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Abbreviations used in the columns

Prof Em	Professor Emeritus	Guest Scholar	Guest Scholar		
Prof	Professor	Guest Res Assoc	Guest Research Associate		
Vis Prof	Visiting Professor	SPD (JSPS)	Special Post-Doctoral		
Assoc Prof	Associate Professor	l í	Research Fellow (JSPS)		
Vis Assoc Prof	Visiting Associate Professor	PD	Post-Doctoral Research Fellow		
Senior Lect	Senior Lecturer	Res	Researcher		
Assist Prof	Assistant Professor	Res Support Staff	Research Support Staff		
Lect (pt)	Lecturer (part-time)	RF	Research Fellow		
Specially Appoint	ed Prof	D 1~3	Doctoral Course (Program) 1~3		
	Specially Appointed Professor	M1~2	Master's Course (Program) 1~2		
Program-Specific	Assoc Prof	RS	Research Student		
	Program-Specific Associate	UG	Undergraduate Student		
	Professor	D Sc	Doctor of Science		
Program-Specific	Senior Lect	D Eng	Doctor of Engineering		
	Program-Specific Senior Lecturer	D Agr	Doctor of Agricultural Science		
Program-Specific	Assist Prof	D Pharm Sc	Doctor of Pharmaceutical Science		
	Program-Specific Assistant	D Med Sc	Doctor of Medical Science		
	Professor	D Inf	Doctor of Informatics		
Techn Staff	Technical Staff	D Human & Envir	D Human & Envirnmtl. Studies		
Program-Specific	Res	1	Doctor of Human and		
	Program-Specific Researcher	1	Environmental Studies		
Proj Res	Project Researcher	D Energy Sc	Doctor of Energy Science		
Support Staff	Support Staff	Ph D	Doctor of Philosophy		
Assist Res Staff	Assistant Research Staff	(pt)	part-time		
Assist Techn Staff	Assistant Technical Staff	 			



Institute for Chemical Research



Topics and introductory columns of laboratories

Division of Synthetic Chemistry - Organoelement Chemistry -

https://www.scl.kyoto-u.ac.jp/~oec/en/index.html



Prof

(D Sc)



Assoc Prof YAMADA, Hiroko MIZUHATA, Yoshiyuki (D Sc)



Assist Prof* MATSUO, Kyohei (D Sc) *New Research Field Development Project



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REN, Zhe (M2) SUZUKI, Shinjiro (M1) TERANISHI, Kento (M1) WANG, Yutang (M1) MIYAZAKI, Kazuya (RS)

Scope of Research

 π -Extended aromatic compounds such as higher acenes and porphyrins are attractive as organic functional materials. In particular, we focus on the control of thin-film structure by self-assembly of the materials to investigate the correlation

between packing structure and charge carrier mobility. We are also interested in the compounds including heavy main group elements to elucidate the similarities and differences in structures and reactivities between organic compounds and the corresponding heavier congeners.

KEYWORDS

Organic Semiconductor Self-Assembly Reactive Intermediate

Aromatic Compound Main Group Element



Recent Selected Publications

Miyazaki, K.; Matsuo, K.; Hayashi, H.; Yamauchi, M.; Aratani, N.; Yamada, H., An Unsymmetrical 5,15-Disubstituted Tetrabenzoporphyrin: Effect of Molecular Symmetry on the Packing Structure and Charge Transporting Property, Org. Lett., 25, 7354-7358 (2023).

Nishino, R.; Tokitoh, N.; Sasayama, R.; Waterman, R.; Mizuhata, Y., Unusual Nuclear Exchange within a Germanium-Containing Aromatic Ring That Results in Germanium Atom Transfer, Nature Commun., 14, 4519 (2023).

Iwai, K.; Mizuhata, Y.; Nakamura, T.; Goto, M.; Wakamiya, A.; Shimakawa, Y.; Tokitoh, N., Solid-State Chromism of Zwitterionic Triarylmethylium Salts, Eur. J. Inorg. Chem., 26, e202300337 (2023).

Jeong, E.; Ito, T.; Takahashi, K.; Koganezawa, T.; Hayashi, H.; Aratani, N.; Suzuki, M.; Yamada, H., Exploration of Alkyl-Group Effects on the Molecular Packing of 5,15-Disubstituted Tetrabenzoporphyrins toward Efficient Charge-Carrier Transport, ACS Appl. Mater. Interfaces, 14, 32319-32329 (2022).

Eimre, K.; Urgel, J. I.; Hayashi, H.; Giovannantonio, M. D.; Ruffieux, P.; Sato, S.; Otomo, S.; Chan, Y. S.; Aratani, N.; Passerone, D.; Gröning, O.; Yamada, H.; Fasel, R.; Pignedoli, C. A., On-Surface Synthesis and Characterization of Nitrogen-Substituted Undecacenes, Nat. Commun., 13, 511 (2022).

Exploration of Alkyl Group Effects on the Molecular Packing of 5,15- Disubstituted Tetrabenzoporphyrins toward Efficient Charge-Carrier Transport

The high design flexibility of organic semiconductors should lead to diverse and complex electronic functions. However, currently available high-performance organic semiconductors are limited in variety; most of p-type materials are based on thienoacenes or related one-dimensionally (1D) extended π -conjugated systems. In an effort to expand the diversity of organic semiconductors, we are working on the development of tetrabenzoporphyrin (BP) derivatives as active-layer components of organic electronic devices. BP derivatives can afford field-effect hole mobilities of >4 cm² V⁻¹ s⁻¹ and the resulting thin films show high thermal stability wherein the field-effect hole mobility stays above 1 cm² V⁻¹ s⁻¹ even after heating at 160 °C in air, reflecting the tight packing of large BP units. These findings will serve as a good basis for extracting the full potential of 2D extended π -frameworks and thus for increasing the structural or functional diversities of high-performance organic semiconductors.

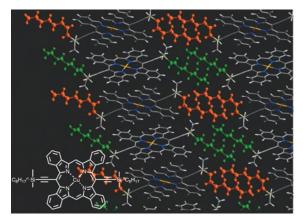


Figure 1. Packing structure of 5,15-bis(*n*-octyldimethylsilylethynyl) tetrabenzoporphyrin in the solution processed thin film.

On-Surface Light-Induced Generation of Higher Acenes and Elucidation of Their Open-Shell Character

Acenes are an important class of polycyclic aromatic hydrocarbons which have recently gained exceptional attention due to their potential as functional organic semiconductors. Fundamentally, they are important systems to study the convergence of physico-chemical properties of all-carbon sp²-frameworks in the one-dimensional limit; and by virtue of having a zigzag edge topology they also provide a fertile playground to explore magnetism in graphenic nanostructures. We have demonstrated the onsurface formation of heptacene and nonacene via visiblelight-induced photo-dissociation of α -bisdiketone precursors on an Au(111) substrate under ultra-high vacuum conditions. Through combined scanning tunneling microscopy/ spectroscopy and non-contact atomic force microscopy investigations, we provide insight into the chemical and electronic structure of these elusive compounds.

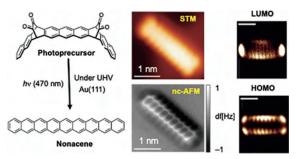


Figure 2. On-surface synthesis of nonacene from photoprecursor and its STM, AFM, and STS images.

Development of Germanium Atom Transfer Reaction

In organic synthesis, the synthetic strategy relies on the division of the target molecule into simpler substructures, the feasibility of which depends on the availability of the necessary building blocks. A single atom is the simplest and most ideal building block for all molecules, but for most elements, obtaining individual atoms for synthesis is impractical. We have demonstrated that single atomic germanium can be introduced into various molecules by taking advantage of the reactivity of the germabenzenyl anion, in which the anionic carbon of the phenyl anion is replaced by germanium. The method discovered in this research enables the controlled synthesis of molecules with "naked" germanium and is expected to lead to the development of various functional materials involving germanium.

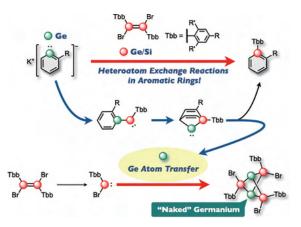


Figure 3. Germanium atom transfer reaction utilizing a germabenzenyl anion.

Division of Synthetic Chemistry - Structural Organic Chemistry -

https://www.scl.kyoto-u.ac.jp/~kouzou/en/index.html



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LIU, Zhibo (D1) SHIMURA, Reo (UG)

Guest Res Assoc

CHAOLUMEN (Ph D)

Inner Mongolia University, P. R. China, 1 August 2023-22 August 2023

Scope of Research

Fundamental studies are being conducted for the creation of new functional π -systems with novel structures and properties, and for evaluation of their application as organic semiconducting materials for photovoltaic and electroluminescent devices. The major subjects are: 1) organochemical transformation of fullerenes C₆₀ and C₇₀, specifically organic

synthesis of endohedral fullerenes by the technique of molecular surgery; 2) generation of ionic fullerene species and their application for the synthesis of functional material; 3) synthesis of new carbon-rich materials by the use of transition metal complex; and 4) creation of new functional π -materials with unique photoelectric properties.

KEYWORDS

 π -Conjugated Systems **Functional Materials** Radical Species

Endohedral Fullerenes Helical Structures

Recent Selected Publications

Zhang, Z.; Murata, Y.; Hirose, T., Circularly Polarized Luminescence of Hetero[n]helicenes with 2,1,3-Thiadiazole Rings at Both Ends: Design of Magnetically-Allowed Electronic Transitions via Heteroatom Embedding, Tetrahedron, 142, 133514 (2023).

Huang, G.; Ide, Y.; Hashikawa, Y.; Hirose, T.; Murata, Y., CH₃CN@open-C₆₀: An Effective Inner-Space Modification and Isotope Effect inside a Nano-Sized Flask, Chem.-Eur. J., 29, e202301161 (2023).

Hashikawa, Y.; Sadai, S.; Murata, Y., Bilateral π-Extension of an Open-[60]Fullerene in a Helical Manner, Chem. Commun., 59, 6560-6563 (2023).

Sadai, S.; Hashikawa, Y.; Murata, Y., π-Extended Open-[70]Fullerenes with a Fused Azaacene, Org. Lett., 25, 2815-2819 (2023). Hashikawa, Y.; Sadai, S.; Okamoto, S.; Murata Y., Near-Infrared-Absorbing Chiral Open [60] Fullerenes, Angew. Chem., Int. Ed., 62, e202215380 (2023).

Near-Infrared-Absorbing Chiral Open-[60] Fullerenes

[60]Fullerene is an achiral molecular nanocarbon with $I_{\rm h}$ symmetry while it could attain an inherent chirality depending upon a functionalization pattern. The conventional chiral induction of C₆₀ relies mainly upon a multiple addition, thus affording a mixture of achiral and chiral isomers. In most cases, however, their chiral function would be largely offset by pseudo-mirror plane(s). These are major obstacles to proceed further study on fullerene chirality and yet leave its understanding elusive. In this study, we developed a carbene-mediated synthesis of C1-symmetric chiral open-[60]fullerenes showing an intense far-red to near-infrared absorption. The large dissymmetry factor of $|g_{abs}| = 0.12$ was confirmed at $\lambda = 820$ nm for circular dichroism in benzonitrile. This is, in general, unachievable by other small chiral organic molecules, demonstrating the potential usage of open-[60]fullerenes as novel types of chiral chromophores.

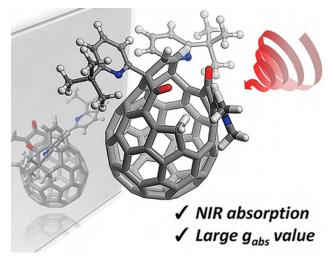


Figure 1. An inherently chiral open-[60] fullerene.

CH₃CN@open-C₆₀: An Effective Inner-Space Modification and Isotope Effect inside a Nano-Sized Flask

The large orifice with a ring-atom count of 18 on a [60] fullerene cage was found to allow for a molecule of CH₃CN to be trapped inside the carbon nanocavity under high-pressure conditions. The thus formed molecular complex exhibited a higher polarity than the empty cage on silica gel, reflecting an increased molecular dipole moment. Furthermore, the encapsulation of CH₃CN caused less negative reductions with respect to empty one, being indic-

ative of a strengthened electron-accepting ability which is mainly attributed to a cage deformation as supported by computational studies. These results are demonstrative of trapped species working as a modulator for external properties of [60]fullerenes from the interior.

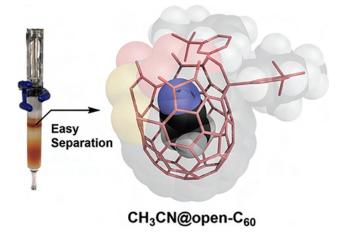


Figure 2. Acetonitrile trapped within a [60]fullerene cage.

Design of Magnetically-Allowed Electronic Transitions by Heteroatom Embedding for an Efficient Circularly Polarized Luminescence (CPL)

Design of excellent circularly polarized luminescence (CPL) emitters requires chiral molecules with large transition magnetic dipole moments (TMDM, $|\mathbf{m}|$). In this work [5]-, [7]-, and [9]helicene derivatives with 2,1,3thiadiazole rings at both ends were designed and synthesized. We revealed that the [9]helicene derivative (**TD**[9] **H**) showed an excellent CPL with a large g_{lum} of +0.04 at 520 nm in toluene, which was significantly larger than that of unsubstituted carbo[7]helicene ($g_{\text{lum}} = +0.008$). Density functional theory (DFT) calculations suggested that the remarkable g_{lum} of **TD**[9]**H** was attributed to the magnetically allowed transition with a large TMDM ($|\mathbf{m}| = 2.3 \times 10^{-20} \text{ erg G}^{-1}$) for the S₁ \rightarrow S₀ transition.

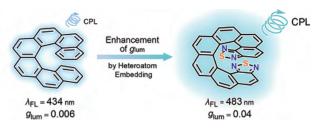


Figure 3. Enhancement of the dissymmetry factor of CPL (g_{lum}) by heteroatom embedding.

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Scope of Research

Our group has been carrying out innovative research on the radical-based organic synthesis by designing catalysts and chemical reactions as well as molecules. Our current research projects include (1) radical-mediated organocatalysis such as N-heterocyclic carbene catalysis or organophotoredox catalysis; (2) radical modification of nucleic acids; and (3) molecular imaging based on boron chemistry.

KEYWORDS

Synthetic Reactions Photoredox Catalysis Organocatalysis Radical Reaction Boron Molecule

Recent Selected Publications

Ota, K.; Nagao, K.; Hata, D.; Sugiyama, H.; Segawa, Y.; Tokunoh, R.; Seki, T.; Miyamoto, N.; Sasaki, Y.; Ohmiya, H., Synthesis of Tertiary Alkylphosphonate Oligonucleotides through Light-Driven Radical-Polar Crossover Reactions, *Nat. Commun.*, **14**, 6856 (2023).

Goto, Y.; Sano, M.; Sumida, Y.; Ohmiya, H., N-Heterocyclic Carbene- and Organic Photoredox-Catalysed meta-Selective Acylation of Electron-Rich Arenes, *Nat. Synth.*, **2**, 1037-1045 (2023).

Nakamura, R.; Yamazaki, T.; Kondo, Y.; Tsukada, M.; Miyamoto, Y.; Arakawa, N.; Sumida, Y.; Kiya, T.; Arai, S.; Ohmiya, H., Radical Caging Strategy for Cholinergic Optopharmacology, J. Am. Chem. Soc., 145, 10651-10658 (2023).

Kodo T.; Nagao K.; Ohmiya H., Organophotoredox-Catalyzed Semipinacol Rearrangement via Radical-Polar Crossover, *Nat. Commun.*, **13**, 2684 (2022).

Nakagawa M.; Matsuki Y.; Nagao K.; Ohmiya H., A Triple Photoredox/Cobalt/Brønsted Acid Catalysis Enabling Markovnikov Hydroalkoxylation of Unactivated Alkenes, J. Am. Chem. Soc., 144, 7953-7959 (2022).

Synthesis of Tertiary Alkylphosphonate Oligonucleotides through Light-Driven Radical-Polar Crossover Reactions

Chemical modification of nucleotides can improve the metabolic stability and target specificity of oligonucleotide therapeutics, and alkylphosphonates have been employed as charge-neutral replacements for naturally-occurring phosphodiester backbones in these compounds. However, at present, the alkyl moieties that can be attached to phosphorus atoms in these compounds are limited to methyl groups or primary/secondary alkyls, and such alkylphosphonate moieties can degrade during oligonucleotide synthesis. The present work demonstrates the tertiary alkylation of the phosphorus atoms of phosphites bearing two 2'deoxynuclosides. This process utilizes a carbocation generated via a light-driven radical-polar crossover mechanism. This protocol provides tertiary alkylphosphonate structures that are difficult to synthesize using existing methods. The conversion of these species to oligonucleotides having charge-neutral alkylphosphonate linkages through a phosphoramidite-based approach was also confirmed in this study.

N-Heterocyclic Carbene- and Organic Photoredox-Catalysed meta-Selective Acylation of Electron-Rich Arenes

meta-Selective functionalization of electron-rich arenes provides a complementary route to that of traditional organic synthesis. In classical electrophilic aromatic substitution reactions of electrondonating group-pendant arenes, C–H functionalization occurs at the *ortho-* or *para*-positions. There have been numerous efforts to overcome this selectivity, and various synthetic methods have been developed, typically using transition metal catalysis. Here we report a combined N-heterocyclic carbene- and organic photoredox-catalysed method for *meta*-selective acylation of electron-rich arenes, using acyl imidazoles as acylating reagents. This approach proceeds without directing groups or steric factors required in transition metal-catalysed processes, resulting in the opposite regioselectivity to conventional approaches such as Friedel–Crafts acylation. Mechanistic studies reveal the process involves a sequence of single-electron oxidation of an electronrich arene followed by the radical–radical coupling between a ketyl radical and an arene radical cation.

Radical Caging Strategy for Cholinergic Optopharmacology

Photo-caged methodologies have been indispensable for elucidating the functional mechanisms of pharmacologically active molecules at the cellular level. A photo-triggered removable unit enables control of the photo-induced expression of pharmacologically active molecular function, resulting in a rapid increase in the concentration of the bioactive compound near the target cell. However, caging the target bioactive compound generally requires specific heteroatom-based functional groups, limiting the types of molecular structures that can be caged. We have developed an unprecedented methodology for caging/uncaging on carbon atoms using a unit with a photo-cleavable carbon-boron bond. The caging/uncaging process requires installation of the CH2-B group on the nitrogen atom that formally assembles an N-methyl group protected with a photoremovable unit. N-Methylation proceeds by photoirradiation via carbon-centered radical generation. Using this radical caging strategy to cage previously uncageable bioactive molecules, we have photocaged molecules with no general labeling sites, including acetylcholine, an endogenous neurotransmitter. Caged acetylcholine provides an unconventional tool for optopharmacology to clarify neuronal mechanisms on the basis of photo-regulating acetylcholine localization. We demonstrated the utility of this probe by monitoring uncaging in HEK cells expressing a biosensor to detect ACh on the cell surface, as well as Ca²⁺ imaging in *Drosophila* brain cells (ex vivo).

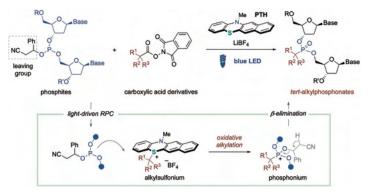
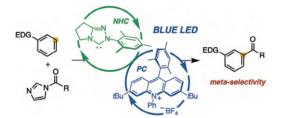


Figure 1. Synthesis of Tertiary Alkylphosphonate Oligonucleotides through Light-Driven Radical-Polar Crossover Reactions.



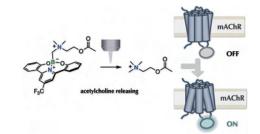


Figure 2. N-Heterocyclic Carbene- and Organic Photoredox-Catalysed meta-Selective Acylation of Electron-Rich Arenes.

Figure 3. Radical Caging Strategy for Cholinergic Optopharmacology.

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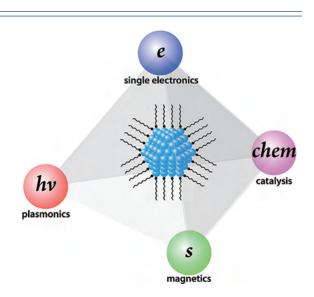
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Scope of Research

We are focusing on the precise synthesis of inorganic nanoparticles by controlling the primary (size, shape, composition, etc.) and secondary (spatial arrangement) structures to tune properties such as electron confinement, carrier oscillation, spin, and catalysis. These high-quality inorganic nanoparticles are applied to both high-performance nanodevices (e.g., single electron transistor, plasmon waveguide, and nanocomposite magnet) and photo-energy conversion materials (e.g., overall water splitting and solar cell).

KEYWORDS

Inorganic Nanomaterials **Oxidation Reduction Reactions** Quantum Dots Plasmonics Photocatalysts



Recent Selected Publications

Endo E.; Saruyama M.; Teranishi T., Location-Selective Immobilisation of Single-Atom Catalysts on the Surface or within the Interior of Ionic Nanocrystals Using Coordination Chemistry, Nat. Commun., 14, 4241 (2023).

Chiga Y.; Takahata R.; Suzuki W.; Mizuhata Y.; Tokitoh N.; Teranishi T, Isomer-Selective Conversion of Au Clusters by Au(I)-Thiolate Insertion. Inorg. Chem., 62, 10049-10053 (2023).

Suzuki W.; Takahata R.; Chiga Y.; Kikkawa S.; Yamazoe S.; Mizuhata Y.; Tokitoh N.; Teranishi T., Control over Ligand-Exchange Positions of Thiolate-Protected Gold Nanoclusters Using Steric Repulsion of Protecting Ligands, J. Am. Chem. Soc., 144, 12310-12320 (2022).

Location-Selective Immobilization of Single-Atom Catalysts on the Surface or Within the Interior of Ionic Nanocrystals Using Coordination Chemistry

Single-atom catalysts dispersed on support materials show excellent heterogeneous catalytic properties that can be tuned using the interactions between the single atoms and the support. Such interactions depend on whether the single atoms are located on the surface or within the interior of the support. However, little is known about immobilising single atoms on the surface or within the interior of supports deliberately and selectively. Herein, such locationselective placement of single atoms is achieved through the choice of metal complex precursor, solvent, and workup procedure. (Figure 1) Using CdSe nanoplatelets as a support, a cis-[PtCl₂(SO(CH₃)₂)₂] precursor in an aprotic solvent exclusively attaches single Pt atoms on the surface of the support. In contrast, a [PtCl₄]₂⁻ precursor in a protic solvent followed by amine treatment places 60% of the single Pt atoms inside the support by cation substitution. The surface-adsorbed single Pt atoms show higher stability in photocatalytic hydrogen evolution than the substituted ones, and the preclusion of substitution as internal Pt maximises the activity. Thus, this study provides a viable strategy for the structurally precise synthesis and design of single-atom catalysts.

Control over Ligand-Exchange Positions of Thiolate-Protected Gold Nanoclusters Using Steric Repulsion of Protecting Ligands

Organic ligands on gold nanoclusters play important roles in regulating the structures of gold cores. However, the impact of the number and positions of the protecting ligands on gold-core structures remains unclear. We isolated thiolate-protected Au₂₅ cluster anions, $[Au_{25}(SC_2Ph)_{17}(Por)_1]^$ and $[Au_{25}(SC_2Ph)_{16}(Por)_2] - (SC_2Ph = 2-phenylethanethiolate),$ obtained by ligand exchange of [Au₂₅(SC₂Ph)₁₈]⁻ with one or two porphyrinthiolate (Por) ligands as mixtures of regioisomers. (Figure 2) The ratio of two regioisomers in $[Au_{25}(SC_2Ph)_{17}(Por)_1]$ - as measured by ¹H NMR spectroscopy revealed that the selectivity could be controlled by the steric hindrance of the incoming thiols. Extended X-ray absorption fine structure studies of a series of porphyrincoordinated gold nanoclusters clarified that the Au13 icosahedral core in the Au₂₅ cluster was distorted through steric repulsion between porphyrin thiolates and phenylethanethiolates. This study reveals interesting insights into the importance of the steric structures of protecting ligands for control over core structures in gold nanoclusters.

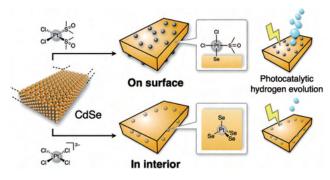


Figure 1. Location-selective immobilization of Pt single atoms on the surface or within the interior of CdSe nanocrystals and its effects on photocatalytic hydrogen evolution.

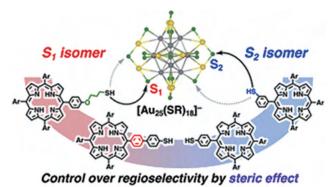


Figure 2. Strategy for control over regioselectivity of $[Au_{25}SR_{18}]^{-}$ by steric effect.

Division of Materials Chemistry – Chemistry of Polymer Materials –

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Scope of Research

We perform kinetic and mechanistic analyses toward understanding chemical and physicochemical reactions occurring in polymerization systems and better routes for synthesis of well-defined polymers. In particular, new well-defined polymers or polymer assemblies are prepared by living polymerization techniques, and their structure-properties relationships

are precisely analyzed. Projects in progress include: 1) kinetics and mechanisms of living radical polymerization (LRP); 2) synthesis of new polymeric materials by living polymerizations and their structure/properties studies; and 3) synthesis, properties, and applications of concentrated polymer brushes (CPB).

KEYWORDS

Precision Polymerization Polymer Brush Hybrid Materials Living Radical Polymerization Tribology



Recent Selected Publications

Nakanishi, Y.; Ishige, R.; Ogawa, H.; Huang, Y.; Sakakibara, K.; Ohno, K.; Kanaya, T.; Takenaka, M.; Tsujii, Y., Unified Explanation for Self-Assembly of Polymer-Brush-Modified Nanoparticles in Ionic Liquids, *Polymer Journal*, **55**, 1199-1209 (2023).

Okubo, H.; Kagiwata, D.; Sasaki, S.; Tsujii, Y.; Nakano, K., Operando Tribo-Raman Spectroscopic Observation for Wear Processes of Superlow Frictional Concentrated Polymer Brushes at Frictional Interface, *Polymer Testing*, **127**, 108170 (2023).

Ishida, K.; Kondo, T., Evaluation of Surface Free Energy Inducing Interfacial Adhesion of Amphiphilic Cellulose Nanofibrils, *Biomacromolecules*, **24**, 3786-3793 (2023).

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Ishida, K.; Kondo, T., Anisotropic Frictional Properties Induced by Cellulose Nanofibril Assembly, Biomacromolecules, 24, 3009-3015 (2023).

Precision Synthesis of Asymmetric Cellulose Nanocrystals with Regioselectively End-Grafted Polymer Brushes

The cellulose nanocrystal (CNC), which is a nanoparticle obtained by hydrolysis of cellulose, has many intriguing properties, including strength, stiffness, biocompatibility, biodegradability, and high aspect ratio. Notably, recent advancements have been made in selectively modifying aldehyde groups located at the reducing edge of CNC with end-grafted polymer chains. Nanoparticles with high-density, concentrated polymer brush (CPB) can form colloidal crystals because of the high resistance against compression and the extremely low friction of the CPB layer. Therefore, we hypothesized that the CNC, with two types of polymers (of different molecular weights) regioselectivity grafted on its reducing edge and other sides (referred to as an asymmetric polymerbrush-modified nanorod: asym-PB nanorod, **Fig. 1**), could form novel higher-order structures because of its asymmetric shape and interparticle repulsive potential.

In this study, we have developed a novel synthetic route for asym-PB nanorods. This involves the introduction of azido groups to the reducing edge of CNC followed by the click reaction to couple reversible addition-fragmentation chain transfer (RAFT) polymerization initiators. Subsequently, atom transfer radical polymerization (ATRP) initiators were introduced to hydroxyl groups on the CNC-side surface to yield a CNC macroinitiator (Fig. 1). Finally, successive RAFT polymerization and ATRP were conducted to obtain the desired asym-PB nanorod. We have confirmed that thus obtained asym-PB nanorod had densely grafted polymer chains at the reducing edge and other CNC-side surface through various evaluations. The surface pressure-area per molecule $(\pi - A)$ isotherms of the asym-PB nanorod showed a distinctive plateau (Fig. 2), suggesting a phase transition occurring possibly thanks to the polymer brush of high molecular weight at the reducing edge. The details studies are now in progress, and our ultimate objective is to create a novel higher-order structure of asym-PB nanorods.



Figure 1. Synthetic scheme for asym-PB nanorod.

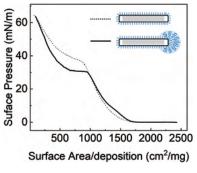


Figure 2. π -A curves for asym-PB nanorod and its analogue.

Hydration Water and Anti-Icing Functions of Hydrophilic Concentrated Polymer Brushes

Hydrophilic concentrated polymer brushes (CPBs) are expected to exhibit antifouling, antifogging, and anti-icing functions, which have been actively studied. To comprehensively understand the mechanism of these functions, it is essential to understand the interaction between CPB and water. However, there are only a few studies on direct measurement of such interactions, and in particular, its analysis and observation at low temperatures, which are important for elucidating the mechanism of the antiicing property, have not yet been accomplished. One of the reasons for this is that CPB is usually an ultra-thin film, making it difficult to apply general-purpose analytical methods. Recently, we succeeded in synthesizing hydrophilic CPBs that are an order of magnitude thicker than previously possible. In this study, we have challenged to directly observe the hydration state of water inside CPB, which had never been achieved before, using CPBs with an ultra-large thickness as the key materials. The results are discussed in relation to the anti-icing property at the CPB interface.

Through the atom transfer radical polymerization of poly (ethylene glycol) methyl ether methacrylate (PEGMA) as a monomer, a hydrophilic CPB with a thickness of about 1 μ m was synthesized on a Si wafer. The ice adhesion strength was measured by horizontally peeling off a cylndrical ice pillar prepared on a surfacemodified Si wafer in a temperature-controlled microscopic stage. The results are shown in **Fig. 3**, suggesting that the effect was above the icephobic level, which is based on 100 kPa or lower. In addition, the hydration state of water-swollen CPB was analyzed by infrared microspectrometry (**Fig. 4**). It was observed that water inside the brush does not freeze even at low temperatures, and this is considered to be responsible for the excellent anti-icing function. Further investigation is currently on-going.

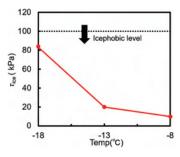


Figure 3. Temperature dependency of ice adhesion strength τ_{ice} for CPB.

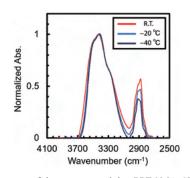


Figure 4. IR spectra of the water-containing PPEGMA-CPB at positions near a water droplet as a function of temperature.

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Scope of Research

Our research focuses on creation of new organic molecules with potential as key reagents and materials for future science and technologies. Furthermore, we have been developing new organic and polymeric materials based on our tailor-made molecules. For example, we are developing a new living radical polymerization method using heavier heteroatom compounds as controlling agents. Another topic is the synthesis of cycloparaphenylenes, hoop-shaped π -conjugated molecules, based on new synthetic strategies. We also study various condensed states of polymers by both static and dynamic methods to understand the relationship between structure and physical properties.

Polymer Synthesis



KEYWORDS

Organic Synthesis

Living Radical Polymerization

Polymer Properties

Curved *n*-Conjugated Molecules

Recent Selected Publications

Jiang, Y.; Kibune, M.; Tosaka, M.; Yamago, S., Practical Synthesis of Dendritic Hyperbranched Polyacrylates and Their Topological Block Polymers by Organotellurium-Mediated Emulsion Polymerization in Water, Angew. Chem. Int. Ed., 62, e202306916 (2023).

Tosaka, M.; Takeuchi, H.; Kibune, M.; Tong, T.; Zhu, N.; Yamago, S., Stochastic Simulation of Controlled Radical Polymerization of Dendritic Hyperbranched Polymers, Angew. Chem. Int. Ed., 62, e202305127 (2023).

Terabayashi, T.; Kayahara, E.; Mizuhata, Y.; Tokitoh, N.; Nishinaga, T.; Kato, T.; Yamago, S., Synthesis of Twisted [n]Cycloparaphenylenes by Alkene Insertion, Angew. Chem. Int. Ed., 62, e202214960 (2023).

Jiang, Y.; Fan, W.; Tosaka, M.; Yamago, S., Controlled Synthesis of High-Molecular-Weight Polystyrene and Its Block Copolymers by Emulsion Organotellurium-Mediated Radical Polymerization, ACS Macro Lett., 11, 1331-1335 (2022).

Imamura, Y.; Yamago, S., Role of Lewis Acids in Preventing the Degradation of Dithioester-Dormant Species in the RAFT Polymerization of Acrylamides in Methanol to Enable the Successful Dual Control of Molecular Weight and Tacticity, Polym. Chem., 12, 5336-5341 (2021).

Stochastic Simulation of Controlled Radical Polymerization Forming Dendritic Hyperbranched Polymers

The formation process of hyperbranched polymers (HBPs) based on the reversible deactivation radical polymerization (RDRP) using a branch-inducing monomer, evolmer, was investigated by stochastic simulation. Our original simulation program successfully reproduced the change of dispersities (Ds) during the polymerization process. Based on the simulation, we found that the observed Ds (=1.5–2) are due to the distribution of the number of branches instead of undesired side reactions. We Further found that the branch structures are well controlled, so the majority of HBPs have structures close to the ideal one (Fig. 1). The simulation also suggested that, if we pay attention to individual molecules, the branch density slightly changes depending on molecular weight. This trend was experimentally confirmed by synthesizing HBPs with an evolmer having a phenyl group and analyzing the signal intensity from multiple detectors in size exclusion chromatography.

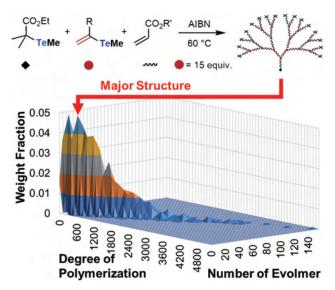


Figure 1. Weight distribution of simulated structure of HBP.

Synthesis of Twisted [*n*]Cycloparaphenylene by Alkene Insertion

By fusing CPP precursors and alkene or ortho-phenylene groups via coupling reactions, mono-alkene-inserted [n] cycloparaphenylenes 1 [(ene)-[n]CPP] with n = 6, 8, and 10, mono-ortho-phenylene-inserted [6]CPP 2, and dialkene-inserted [n]CPP 3 [(ene)₂-[n]CPP] with n = 4, 6, and 8 were synthesized. Single-crystal X-ray diffraction analyses revealed that the strips formed by the π -surfaces of 1 and 2 exhibited a Möbius topology in the solid state. The Möbius topology in the parent 1 and 2 in a solution was lost due to the free rotation of the paraphenylene unit even at low temperatures. On the other hand, ene- [6]CPP 4 with eight 1-pyrrolyl groups preserved the Möbius topology even in a solution. Despite a twist, 1 has in-plane conjugation and possesses a unique size dependence of the electronic properties; i.e., the opposite size dependency of the HOMO-LUMO energy relative to conventional π -conjugated molecules.

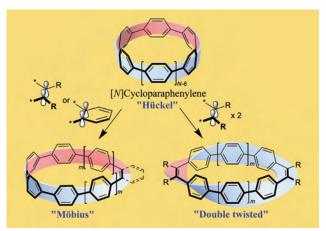


Figure 2. Insertion of alkene or ortho-phenylene units into a CPP skeleton.

Division of Materials Chemistry – Inorganic Photonics Materials –

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Scope of Research

NV centers in diamond have been extensively interested because a single spin of the NV center can be manipulated and detected at room temperature. Furthermore, a spincoherence time of the NV center is very long. The spincoherence time is the time to retain coherence (superposition state) and directly relates to the sensitivity of sensors of magnetic field, electric field and temperature. Therefore, the unique and excellent properties of the NV center are expected to be applied for quantum computing, quantum communication, bio-imaging, and high-sensitive sensor with nano-scale resolution.

KEYWORDS

Diamond Quantum Materials NV Center Quantum Sensing Quantum Information Science



Recent Selected Publications

Fujiwara, M.; Fu, H.; Hariki, N.; Ohki, I.; Makino, Y.; Liu, M.; Tsurui, A.; Yoshikawa, T.; Nishikawa, M.; Mizuochi, N., Germanium-Vacancy Centers in Detonation Nanodiamond for All-Optical Nanoscale Thermometry, *Appl. Phys. Lett.*, **123**, 181903 (2023). Morishita, H.; Morioka, N.; Nishikawa, T.; Yao, H.; Onoda, S.; Abe, H.; Ohshima, T.; Mizuochi, N., Spin-Dependent Dynamics of Photocarrier

Generation in Electrically Detected Nitrogen-Vacancy-Based Quantum Sensing, *Phys. Rev. Appl.*, **19**, 034061 (2023).

Fujiwara, M.; Inoue, S.; Masuno, S.; Fu, H.; Tokita, S.; Hashida, M.; Mizuochi, N., Creation of NV Centers over a Millimeter-Sized Region by Intense Single-Shot Ultrashort Laser Irradiation, *APL Photonics*, **8**, 036108 (2023).





(Ph D)

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Ultra-Long Coherence Times Amongst Room-Temperature Solid-State Spins

Solid-state single spins are promising resources for quantum sensing, quantum-information processing and quantum networks, because they are compatible with scalable quantum-device engineering. However, the extension of their coherence times proves challenging. Although enrichment of the spin-zero ¹²C and ²⁸Si isotopes drastically reduces spin-bath decoherence in diamond and silicon, the solid-state environment provides deleterious interactions between the electron spin and the remaining spins of its surrounding. Here we demonstrate, contrary to widespread belief, that an impurity-doped (phosphorus) n-type singlecrystal diamond realises remarkably long spin- coherence times. Single electron spins show the longest inhomogeneous spin-dephasing time ($T_2^* \approx 1.5 \text{ ms}$) and Hahn-echo spin-coherence time ($T_2 \approx 2.4$ ms) ever observed in room-temperature solid-state systems, leading to the best sensitivities (amongst others such as temperature), which we confirmed for AC magnetic fields. From the analysis of the noise spectrum, the elongation of T₂ could be realised by optimising the phosphorus concentration and by continuing to decrease the paramagnetic impurities and defects.

The extension of coherence times in diamond semiconductor may allow for new applications in quantum technology.

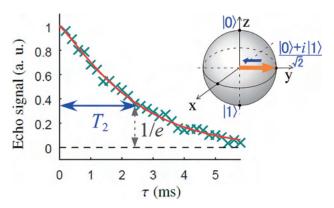


Figure 1. Echo signal of the single NV centre at room temperature. (Insert) Bloch sphere to show the coherence (superposition state).

Extension of the Coherence Time by Generating MW Dressed States in a Single NV Centre in Diamond

Nitrogen-vacancy (NV) centres in diamond hold promise in quantum sensing applications. A major interest in them is an enhancement of their sensitivity by the extension of the coherence time (T_2) . In this report, we experimentally generated more than four dressed states in a single NV centre in diamond based on Autler-Townes splitting (ATS). We also observed the extension of the coherence time to $T_2 \sim 1.5$ ms which is more than two orders of magnitude longer than that of the undressed states. Numerical estimations show the sensitivity of the quantum sensing with the dressed states can be enhanced at least one-order of magnitude with experimentally observed T_{20} and T_2 . Thus, we believe that the quantum sensing with the dressed states can be applicable for improving the sensitivity of a quantum sensing. As an example of a quantum application using these results we propose a protocol of quantum sensing, which shows more than an order of magnitude enhancement in the sensitivity.

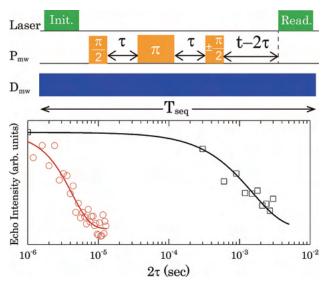


Figure 2. (Top) Pulse sequence to observe $T_{2\rho}$ and T_2 with applying a phase cycle to the final $\pi/2$ pulse. (Bottom) Black and red plots show the results of $T_{2\rho}$ and T_2 measurements, respectively. They are fitted by exponential decay curves described by black and red solid lines.

Division of Materials Chemistry - Nanospintronics -

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Scope of Research

Conventional electronics uses only the charge of electrons, while traditional magnetic devices use only the spin degree of freedom of electrons. Aiming at complete control of both charge and spin in single solid-state devices, an emerging field called spintronics is rapidly developing and having an impact on information technologies. By combining the atomic-layer deposition with nanofabrication, we focus on the development of spin properties of various materials and the control of quantum effects in mesoscopic systems for novel spintronics devices.



KEYWORDS

Spintronics Magnetism Magnetic Materials

Recent Selected Publications

Narita, H.; Ishizuka, J.; Kan, D.; Shimakawa, Y.; Yanase, Y.; Ono, T., Magnetization Control of Zero-Field Intrinsic Superconducting Diode Effect, Adv. Mater., 35, 2304083 (2023).

Moriyama, T.; Sanchez-Tejerina, L.; Oda, K.; Ohkochi, T.; Kimata, M.; Shiota, Y.; Nojiri, H.; Finocchio, G.; Ono, T., Micromagnetic Understanding of Evolutions of Antiferromagnetic Domains in NiO, Phys. Rev. Mater., 7, 054401 (2023).

Hayashi, D.; Shiota, Y.; Ishibashi, M.; Hisatomi, R.; Moriyama, T.; Ono, T., Observation of Mode Splitting by Magnon-Magnon Coupling in Synthetic Antiferromagnets, Appl. Phys. Express, 15, 053004 (2023).

Hisatomi, R.; Taga, K.; Sasaki, R.; Shiota, Y.; Moriyama, T.; Ono, T., Quantitative Optical Imaging Method for Surface Acoustic Waves Using Optical Path Modulation, Phys. Rev. B, 107, 165416 (2023).

Ham, W. S.; Ho T. H.; Shiota, Y.; Iino, T.; Ando, F.; Ikebuchi, T.; Kotani, Y.; Nakamura, T.; Kan, D.; Shimakawa, Y.; Moriyama, T.; Im, E.; Lee, N. J.; Kim, K. W.; Hong, S. C.; Rhim, S. H.; Ono, T.; Kim, S., Generation of Spin-Polarized Electronic Currents Using Perpendicularly Magnetized Cobalt Ferrite Spin-Filtering Barriers Grown on Spinel-Type-Conductive, Adv. Sci., 10, 2206800 (2023).

Realization of the Field-Free Superconducting Diode Effect

The diode effect is fundamental to electronic devices and is widely used in rectifiers and AC-DC converters. At low temperatures, however, conventional semiconductor diodes possess a high resistivity, which yields energy loss and heating during operation. The superconducting diode effect (SDE), which relies on broken inversion symmetry in a superconductor may mitigate this obstacle: in one direction a zeroresistance supercurrent can flow through the diode, but for the opposite direction of current flow, the device enters the normal state with ohmic resistance. The application of a magnetic field can induce SDE in Nb/V/Ta superlattices with a polar structure, in superconducting devices with asymmetric patterning of pinning centres, or in superconductor/ferromagnet hybrid devices with induced vortices. The need for an external magnetic field limits their practical application. Here, we present implementation of zero-field SDE using noncentrosymmetric [Nb/V/Co/V/Ta]20 multilayers. The magnetic layers provide the necessary symmetry breaking and we can tune the SDE by adjusting the structural parameters, such as the constituent elements, film thickness, stacking order, and number of repetitions. We control the polarity of the SDE through the magnetization direction of the ferromagnetic layers. Energyloss-free SDEs as presented in this work may therefore enable novel non-volatile memories and logic circuits with ultralow power consumption.

Spin-Transfer-Torque-Driven Magnetic Domain Wall Motion in Antiferromagnetically Coupled Ferrimagnets

Magnetic domain wall (DW) racetrack memory is a next-generation, non-volatile and high-density magnetic memory, where the magnetic domain walls work as information bits and they are controlled by electric current via the effect of spin transfer torque (STT). However, to enhance thermal stability while keeping low driven current is difficult in traditional domain wall (DW) motion devices. The increasing of energy barrier for thermal stability inevitably results in the enhancement of driven current. We numerically investigate depinning field (H_{depin}) and critical current density (J_c) for DW motion as a function of uniaxial magnetic anisotropy (K_u) in vertical DW motion memory with artificial ferromagnet. It is found that H_{depin} and J_c show different K_u dependence. The results indicate that it is promising to simultaneously achieve high thermal stability and low driven current in artificial ferromagnet based DW motion devices.

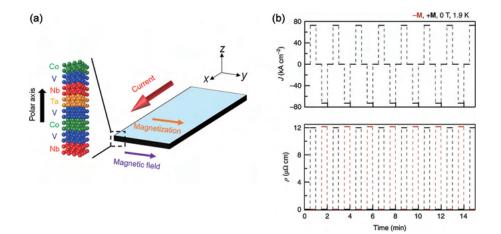


Figure 1. (a) Schematic of the SDE and measurement configuration. The magnetic field is applied perpendicular to both the polar axis and the electrical current. (b) Non-volatile SDE at 1.9 K. Red and black dots represent the results for negative magnetization (-**M**) and positive magnetization (+**M**), respectively. Current densities J = 72.7 kA cm⁻² and J = -72.7 kA cm⁻² at 1.9 K without a magnetic field were repeatedly applied. The device shows a superconducting state or normal conducting state depending on the polarity of the current. Note that the polarity of SDE depends on the direction of magnetization. The -**M** or +**M** state is achieved after sweeping the magnetic field in the order of +0.5, 0, -0.15, 0 T or -0.5, 0, +0.15, 0 T.

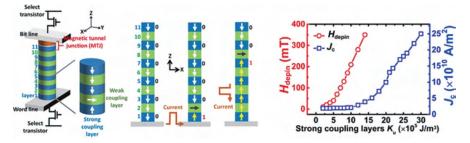


Figure 2. (a) Schematic illustration of the experimental setup. (b) The STT-induced DW velocity as a function of temperature. The dotted orange line represents the angular momentum compensation temperature T_A .

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Scope of Research

The ultimate goal of our research is the regulation of cellular functions by designed peptides and proteins. Current research subjects include (1) development of novel intracellular delivery systems aiming at elucidation and control of cellular functions using designed membrane permeable peptide vectors, (2) elucidation of the DNA or RNA binding modes of nucleic acid binding proteins, and design of artificial regulators of gene expression, (3) elucidation and control of membrane curvature, and (4) design of stimulation-responsible artificial peptides and proteins.



KEYWORDS

Membrane-Permeable Peptides Intracellular Delivery Peptide Design DNA/RNA Binding Protein Membrane Curvature

Recent Selected Publications

Hirose H.; Nakata E.; Zhang Z.; Shibano Y.; Maekawa M.; Morii T.; Futaki, S., Macropinoscope: Real-Time Simultaneous Tracking of pH and Cathepsin B Activity in Individual Macropinosomes, Anal. Chem., 95, 11410-11419 (2023).

Tanaka K.; Suda A.; Uesugi M.; Futaki S.; Imanishi M., Xanthine Derivatives Inhibit FTO in an L-ascorbic Acid-Dependent Manner, Chem. Commun., 59, 10809-10812 (2023).

Omura M.; Morimoto K.; Araki Y.; Hirose H.; Kawaguchi Y.; Kitayama Y.; Goto Y.; Harada A.; Fujii I.; Takatani-Nakase T.; Futaki S.; Nakase I., Inkjet-Based Intracellular Delivery System that Effectively Utilizes Cell-Penetrating Peptides for Cytosolic Introduction of Biomacromolecules through the Cell Membrane, ACS Appl. Mater Interfaces, 15, 47855-47865 (2023).

Nishimura M.; Kawaguchi Y.; Kuroki K.; Nakagawa Y.; Masuda T.; Sakai T.; Kawano K.; Hirose H.; Imanishi M.; Takatani-Nakase T.; Afonin S.; Ulrich A. S.; Futaki S., Structural Dissection of Epsin-1 N-Terminal Helical Peptide: The Role of Hydrophobic Residues in Modulating Membrane Curvature, Chemistry, 29, e202300129 (2023).

Hirose H.; Maekawa M.; Ida H.; Kuriyama M.; Takahashi Y.; Futaki S., A Noncanonical Endocytic Pathway is Involved in the Internalization of 3 µm Polystyrene Beads into HeLa Cells, Bioconjug. Chem., 33, 1851-1859 (2022).

Development of a Dual Sensor to Track pH and an Enzyme Activity in Individual Macropinosomes

Macropinocytosis is an endocytic pathway that results in the formation of macropinosomes through massive uptake of extracellular fluids. For instance, certain cancer cell types use macropinocytosis to obtain extracellular nutrients, such as amino acids, to support their proliferation. Furthermore, macropinocytosis represents a promising route for the effective delivery of biological macromolecules including proteins and antibodies. Nonetheless, a comprehensive understanding of the intracellular dynamics of macropinosomes has yet to be attained. Increased knowledge of individual macropinosomes behavior in living cells could significantly impact the design concept of drug delivery tools and development of drugs against cancer.

A fluorescent sensor that enables simultaneous analysis of multiple parameters in limited or specific cellular space is useful for comprehending molecular dynamics and biological responses in living cells. In this study, we aimed to develop a macropinoscope, a fluorescent sensor that detects both pH and cathepsin B activity in individual macropinosomes through fluorescence microscopy. Dextran (70 kDa) was utilized as a macropinosomespecific marker platform, onto which three fluorophores (fluorescein, Oregon Green, and tetramethylrhodamine) were loaded for ratiometric pH sensing and imaging. Additionally, a cathepsin-B-cleavable peptide sequence, bearing sulfo-Cy5 fluorophore and the BHQ-3 quencher, was loaded onto the platform. The cathepsin B activity can be detected by an increase in sulfo-Cy5 fluorescence when the peptide sequence is cleaved. The macropinoscope was utilized to investigate the behavior of individual macropinosomes produced by constitutive macropinocytosis in HT1080 cells. We discovered that a sharp decrease in pH occurred close to the cell nucleus, 5-10 minutes after macropinosome formation. We also observed an immediate rise in cathepsin B activity as the pH of the macropinosome reached around 6.

In the future, the sensor is expected to enable thorough examination of macropinosome behavior under other conditions and in different cell types. Additionally, our design concept will pave the way for the development of various macropinoscopes tailored to other parameters in individual macropinosomes.

Reference

[1] Hirose, H. et al., Anal. Chem. 95, 11410-11419 (2023).

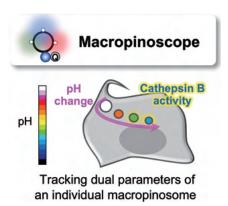


Figure 1. Macropinoscope can track dual parameters (pH and cathepsin B activity) of individual macropinosomes by fluorescence microscopy. Reprinted from [1].

Inhibition of m⁶A Demethylation Activity of FTO by Xanthine Derivatives with L-Ascorbic Acid-Related Manner

Chemical modifications of RNA play an important role in gene regulation. In particular, N⁶-methyladenosine (m⁶A), which is present in transcripts at high frequency, is involved in development and differentiation as well as various diseases. Despite the increasing evidence of the importance of m6A RNA methylation, convenient m⁶A detection methods for measuring the activity of RNA methyltransferases and demethylases and for screening their inhibitors have been lacking. Here, a simple method to detect the methylation states of RNA was constructed using the Escherichia coli RNA endonuclease MazF, which we found to be m⁶A-sensitive, in combination with the FRET probe containing an m⁶A consensus RNA sequence. We searched for inhibitors of the m⁶A demethylase FTO, one of the member of Fe(II) and 2oxoglutarate-dependent oxygenases. Xanthine derivatives were identified as specific inhibitors of the m6A demethylase activity of FTO. These inhibitors exhibited L-ascorbic acid concentrationdependent inhibitory activity against FTO, an unprecedented mode of inhibition. Our results have significant implications for understanding the regulatory mechanisms of FTO and the design of FTO-specific inhibitors.

Reference

[2] Tanaka, K. et al., Chem. Commun. 59, 10809-10812 (2023).

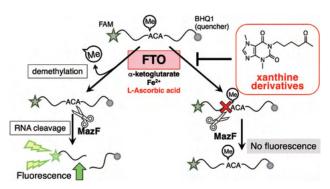


Figure 2. An activity-based screening for FTO inhibitor identified xanthine derivatives as specific inhibitor with an L-ascorbic acid-dependent mode of inhibition. Reprinted from [2].

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Assist Prof Prof YAMAGUCHI, Shinjiro MASHIGUCHI, Kiyoshi (D Agr) (D Agr)



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*Qingdao Agricultural University, China, 1 November 2022-31 October 2023

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Scope of Research

Plant hormones are a group of small molecules that are synthesized by plants and control their growth, development and environmental responses. This laboratory aims at elucidating how plant hormones are made and act in plants. Towards this goal, we combine chemical (organic chemistry, biochemistry, and analytical chemistry) and biological (molecular genetics, physiology, molecular biology, genomics) approaches. We are also looking for new hormone-like compounds by using mutant plants that show morphological phenotypes.

KEYWORDS

Plant Hormone Strigolactone Biosynthesis Cytochrome P450 Receptor



Recent Selected Publications

Mashiguchi, K.; Morita, R.; Tanaka, K.; Kodama, K.; Kameoka, H.; Kyozuka, J.; Seto, Y.; Yamaguchi, S., Activation of Strigolactone Biosynthesis by the DWARF14-LIKE/KARRIKIN-INSENSITIVE2 Pathway in Mycorrhizal Angiosperms, but Not in Arabidopsis, a Non-Mycorrhizal Plant, Plant Cell Physiol., 64, 1066-1078 (2023).

Cui, J.; Nishide, N.; Mashiguchi, K.; Kuroha, K.; Miya, M.; Sugimoto, K.; Itoh, J.-I.; Yamaguchi, S.; Izawa, T., Fertilization Controls Tiller Numbers via Transcriptional Regulation of a MAXI-like Gene in Rice Cultivation, Nat. Commun., 14, 3191 (2023).

Mashiguchi, K.; Seto, Y.; Onozuka, Y.; Suzuki, S.; Takemoto, K.; Wang, Y.; Dong, L.; Asami, K.; Noda, R.; Kisugi, T.; Kitaoka, N.; Akiyama, K.; Bouwmeester, H.; Yamaguchi, S., A Carlactonoic Acid Methyltransferase That Contributes to the Inhibition of Shoot Branching in Arabidopsis, Proc. Natl. Acad. Sci. U.S.A., 119(14), e2111565119 (2022).

Ishida, T.; Watanabe, B.; Mashiguchi, K.; Yamaguchi, S., Synthesis and Structure-Activity Relationship of 16,17-Modified Gibberellin Derivatives, Phytochem Lett., 49, 162-166 (2022).

Mashiguchi, K.; Seto, Y.; Yamaguchi, S., Strigolactone Biosynthesis, Transport and Perception, Plant J., 105, 335-350 (2021).

The Mechanism for Strigolactone Perception and Deactivation by a DWARF14 Receptor

Strigolactones (SLs) have been identified as root-derived signals for parasitic and symbiotic interactions in the rhizosphere. In addition to these functions as allelochemicals, SLs are now known as endogenous plant hormones that regulate many aspects of plant growth such as outgrowth of axillary shoots, root development and leaf senescence.

Recently, the perception mechanism for SLs has been a subject of debate because their receptor, DWARF14 (D14), is an α/β -hydrolase that can cleave SLs. In the study of Seto *et al.* (2019), we first conducted time-course analyses of SL binding and hydrolysis by Arabidopsis D14 (AtD14) by using differential scanning fluorimetry (DSF) experiments and hydrolysis assays (Figure 1). In these analyses, we found that the level of uncleaved GR24, a synthetic SL analog, strongly correlates with the induction of the melting temperature (Tm) shift of AtD14, suggesting that SLs trigger the active state of D14 before their hydrolysis.

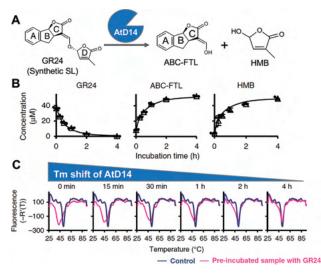


Figure 1. The time-course analyses of SL binding and hydrolysis by AtD14. (A) Hydrolysis reaction of SL (GR24) by AtD14. (B) Quantification of the hydrolysis reaction of GR24 (40 μ M) by AtD14. (C) The Tm shift of AtD14 incubated with GR24 (40 μ M) in DSF analysis. The maximum Tm shift was observed at initial incubation (0 min).

We next analyzed the catalytic triad mutants of AtD14. Among them, interestingly, the AtD14^{D218A} mutant completely complemented the hyper-branching phenotype of the *atd14* mutant though it lacks the hydrolase activity (Figure 2). Moreover, we found that the AtD14^{D218A} mutant could interact with SMXL7, a negative regulator of SL signaling, in an SL-dependent manner in yeast two hybrid experiments (Figure 2). These findings suggest that the hydrolase reaction catalyzed by D14 is not necessary for the signal transducing role.

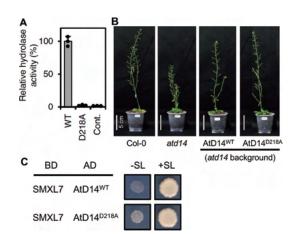


Figure 2. Functional analysis of the AtD14^{D218A} mutant. (A) The SL hydrolysis activities of maltose binding protein (MBP)-tagged wild-type of AtD14 protein (AtD14^{WT}) and the AtD14^{D218A} mutant. MBP was used in the control reaction. (B) The branching phenotype of Arabidopsis transgenic plants expressing AtD14^{WT} and AtD14^{D218A}. (C) The SL-dependent interaction of SMXL7 with AtD14^{WT} and AtD14^{D218A} in yeast.

Moreover, we showed that overexpression of the AtD14^{R183H} mutant, which could not interact with SMXL7 in the presence of SLs, but could hydrolyze SLs like AtD14^{WT}, resulted in an increased shoot branching phenotype (data not shown). These results support the idea that the hydrolase reaction catalyzed by D14 would be a deactivating step of SLs after transducing the signal.

From these lines of evidence, we conclude that the intact SL molecules trigger the D14 active signaling state, and that D14 deactivates bioactive SLs by hydrolysis after signal transmission. Together, our results revealed that D14 is a dual-functional receptor, responsible for both the perception and deactivation of bioactive SLs (Figure 3).

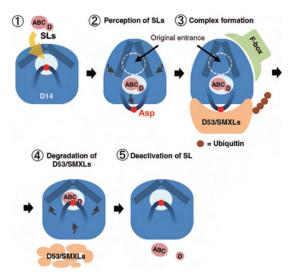


Figure 3. A proposed model of D14 in SL signaling. Bioactive SLs induce the conformational changes of D14, which triggers complex formation with the signaling partners. After the degradation of negative regulators of SL signaling (D53/SMXLs) and transmission of the SL signal, D14 reconstructs the catalytic triad to inactivate the bioactive SL.

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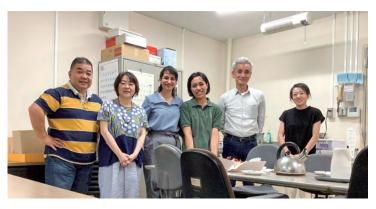
RUBIO, Vicente (Ph D) GALBIATI, Massimo (Ph D) Centro Nacional de Biotecnologia, CSIC, Spain, 6 October 2023–14 October 2023 Institute of Agricultural Biology and Biotechnology, CNR, Italy, 17 November 2023– 28 November 2023

Scope of Research

This laboratory aims at clarifying molecular bases of regulatory mechanisms for plant development, especially plant morphogenesis, with techniques of forward and reverse genetics, molecular biology, and biochemistry. Current major subjects are: 1) phospholipid signaling in cell morphogenesis, 2) transcriptional network for cell morphogenesis, 3) COP9 signalosome modulating signal transduction in the nuclei, and 4) RNA processing mediated gene expression regulation.

KEYWORDS

Morphogenesis Phospholipid Signaling mRNA Processing Signal Transduction COP9 Signalosome



Recent Selected Publications

Kato, M.; Watari, M.; Tsuge, T.; Zhong, S.; Gu, H.; Qu, L.-J.; Fujiwara, T.; Aoyama, T., Redundant Function of the *Arabidopsis* Phosphatidylinositol 4-Phosphate 5-Kinase Genes *PIP5K4-6* is Essential for Pollen Germination, *Plant J.*, (in press).

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Zhang, X.; Nomoto, M.; Garcia-León, M.; Takahashi, N.; Kato, M.; Yura, K.; Umeda, M.; Rubio, V.; Tada, Y.; Furumoto, T.; Aoyama, T.; Tsuge, T., CFI 25 Subunit of Cleavage Factor I is Important for Maintaining the Diversity of 3' UTR Lengths in *Arabidopsis thaliana* (L.) Heynh, *Plant Cell Physiol.*, **63**, 369-383 (2022).

Redundant Function of the *Arabidopsis* **PIP5K Genes for Pollen Germination**

Pollen is the male gametophyte with a functional structure for transferring sperm cells to the egg apparatus in seed plants. Pollen undergoes unique cell biological processes of pollen development to support its structural development and functional performance. After pollination, a pollen grain first establishes a cell polarity focusing on the future germination site, and then, a pollen tube germinates and elongates through tip growth toward the embryo sac according to a series of guidance signals. Although these complicated processes accurately progress, underlying regulatory mechanisms remain largely elusive, especially for the germination process involving the cell polarity.

Phosphatidylinositol 4,5-bisphosphate [PtdIns(4,5) P_2], one of phosphoinositides serving as a signaling molecule in eukaryotic cells is localized mainly to the plasma membrane frequently with a polarized pattern. Through the functions of its interacting proteins, PtdIns(4,5) P_2 regulates various cell biological processes, including cytoskeletal organization, membrane trafficking, and signal transduction for gene expression. While the metabolic pathways of phosphoinositides link together to form a complicated network, the phosphorylation of PtdIns(4)P by phosphatidylinositol 4-phosphate 5-kinase (PIP5K) is thought to be a key pathway responsible for the production of PtdIns(4,5) P_2 in higher plants, where some of the phosphoinositide metabolic pathways found in animals or fungi are missing.

Among the 11 PIP5K genes of Arabidopsis thaliana, PIP5K4, PIP5K5, and PIP5K6 have been intensively studied on their functions in pollen tube growth, and strongly suggested to have an indispensable function for the elaborate pollen system of angiosperms. However, this idea remains to be verified, mainly because comprehensive genetic analysis of the genes using their loss-of-function mutants has not been done. We performed a comprehensive genetic analysis of the genes and revealed that their redundant function is essential for pollen germination. Pollen with the *pip5k4pip5k5pip5k6* triple mutation was sterile. PIP5K4-YFP, PIP5K5-YFP, and PIP5K6-YFP, which could rescue the sterility of the triple mutant pollen, preferentially localized to the tricolpate aperture area and the future germination site on the plasma membrane prior to germination (Figure 1). Triple mutant pollen grains under the germination condition, in which spatiotemporal localization of the PtdIns $(4,5)P_2$ fluorescent marker protein 2xmCHERRY-2xPH^{PLC} as seen in the wild type was abolished (Figure 2), exhibited swelling and rupture of the pollen wall, but neither the conspicuous protruding site nor site-specific deposition of cell wall materials for germination. These data indicate that PIP5K4-6 and their product PtdIns $(4,5)P_2$ are essential for pollen germination, possibly through the establishment of the germination polarity in a pollen grain.

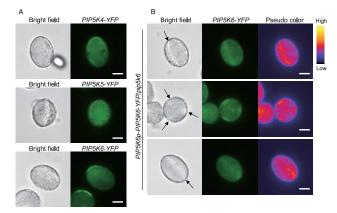


Figure 1. Subcellular localization of YFP-fused PIP5K4–6 proteins prior to pollen germination. (A) Bright field (left) and YFP fluorescence (right) images of pollen grains expressing PIP5K4-YFP, PIP5K5-YFP, and PIP5K6-YFP prior to pollen germination are shown. (B) Bright field (left) and YFP fluorescence (middle) images, and index-color images of YFP fluorescence (right) of pollen grains expressing PIP5K6-YFP prior to pollen germination are shown. Arrows on bright field images in (A) indicate pollen apertures. Scale bars: 10 μm.

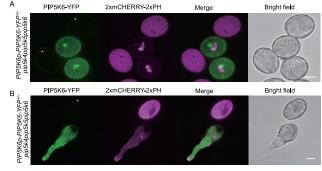


Figure 2. Subcellular localization of PtdIns(4,5)P₂ marker protein and PIP5K6-YFP in the *pip5k4 pip5k5 pip5k6*⁻ pollen. Pollen grains from transgenic plants heterozygously and homozygously containing *PIP5K6p*-*PIP5K6-YFP* and *UBQ10p-2xmCHERRY-2xPH^{PLC}*, respectively, in the *pip5k4pip5k5pip5k6* background were untreated (A) or treated (B) with pollen germination medium. Fluorescence images of PIP5K6-YFP (left) and 2xmCHERRY-2xPH^{PLC} (second left), merged images (second right), and bright field images (right) are shown. Asterisks indicate *pip5k4pip5k5pip5k6* pollen grains without the *PIP5K6p-PIP5K6-YFP* transgene. Scale bars: 10 µm.

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Scope of Research

Chemical biology is an interdisciplinary field of study that is often defined as "chemistry-initiated biology." As biological processes all stem from chemical events, it should be possible to understand or manipulate biological events using chemistry. Our laboratory has been discovering or designing unique organic molecules that modulate fundamental processes in human cells. Such synthetic organic molecules often serve as tools for basic cell biology. Discovery or design of small molecules with unique biological activities permits small-molecule-initiated exploration of complex cellular events.

Our mission is to create a new world of bioactive synthetic molecules: new modes of activity, new shapes, and new sizes. We hope that these basic studies open new avenues for small-molecule applications in a range of fields.

KEYWORDS

Chemical Biology **Chemical Genetics** Self-Assembly Chemical Library Immunology

Recent Selected Publications

Perron, A.; Mandal, S.; Chuba, T.; Mao, D.; Singh, V.; Noda, N.; Tan, R.; Vu, H.; Abo, M.; Uesugi, M., Small-Molecule Drug Repurposing for Counteracting Phototoxic A2E Aggregation, ACS Chem. Biol., 18(10), 2170-2175 (2023).

Zhuo, S.; Noda, N.; Hioki, K.; Jin, S.; Hayashi, T.; Hiraga, K.; Momose, H.; Li, W.; Zhao, L.; Mizukami, T.; Ishii, K.; Li, Y.; Uesugi, M., Identification of a Self-Assembling Small-Molecule Cancer Vaccine Adjuvant with an Improved Toxicity Profile, J. Med. Chem., 66(18), 13266-13279 (2023).

Toh, K.; Nishio, K.; Nakagawa, R.; Egoshi, S.; Abo, M.; Perron, A.; Sato, S.; Okumura, N.; Koizumi, N.; Dodo, K.; Sodeoka, M.; Uesugi, M., Chemoproteomic Identification of Blue-Light-Damaged Proteins, J. Am. Chem. Soc., 144, 20171-20176 (2022).

Jin, S.; Zhuo, S.; Takemoto, Y.; Li, Y.; Uesugi, M., Self-Assembling Small-Molecule Adjuvants as Antigen Nano-Carriers, Chem Commun., 58, 12228-12231 (2022).

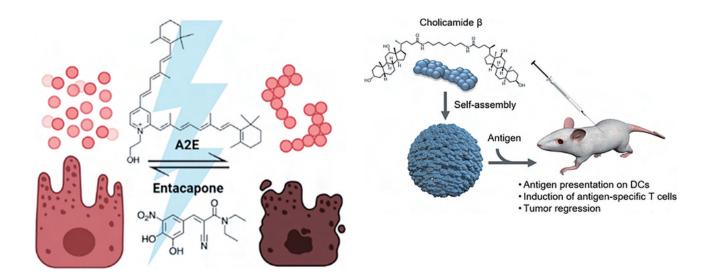
Nishio, K.; Toh, K.; Perron, A.; Goto, M.; Abo, M.; Shimakawa, Y.; Uesugi, M., Magnetic Control of Cells by Chemical Fabrication of Melanin, J. Am. Chem. Soc., 144, 16720-16725 (2022).

Small-Molecule Drug Repurposing for Counteracting Phototoxic A2E Aggregation

Despite the well-established role of oxidative stress in the pathogenesis of age-related macular degeneration (AMD), the mechanism underlying phototoxicity remains unclear. The Uesugi group used a drug repurposing approach to isolate an FDA-approved drug that blocks the aggregation of the photoinducible major fluorophore of lipofuscin, bis-retinoid N-retinylidene-N-retinylethanolamine the (A2E). Their fluorescence-based screening combined with dynamic light scattering (DLS) analysis led to the identification of entacapone as a potent inhibitor of A2E fluorescence and aggregation. The entacapone-mediated inhibition of A2E aggregation blocks its photodegradation and offers photoprotection in A2E-loaded retinal pigment epithelial (RPE) cells exposed to blue light. In-depth mechanistic analysis suggests that entacapone prevents the conversion of toxic aggregates by redirecting A2E into off-pathway oligomers. These findings provide evidence that aggregation contributes to the phototoxicity of A2E.

Identification of a Self-Assembling Small-Molecule Cancer Vaccine Adjuvant with an Improved Toxicity Profile

Protein or peptide cancer vaccines usually include immune potentiators, so-called adjuvants. However, it remains challenging to identify structurally simple, chemically accessible synthetic molecules that are effective and safe as vaccine adjuvant. The Uesugi group discovered cholicamide β (6), a self-assembling small-molecule vaccine adjuvant with an improved toxicity profile and proven efficacy in vivo. The Uesugi group and their collaborators demonstrated that cholicamide β (6), which is less cytotoxic than its parent compound, forms virus-like particles to potently activate dendritic cells with the concomitant secretion of cytokines. When combined with a peptide antigen, cholicamide β (6) potentiated the antigen presentation on dendritic cells to induce antigen-specific T cells. As a therapeutic cancer vaccine adjuvant in mice, a mixture of cholicamide β (6) and a peptide antigen protected mice from the challenges of malignant cancer cells without overt toxicity. Cholicamide β (6) may offer a translational opportunity as an unprecedented class of small-molecule cancer vaccine adjuvants.



Division of Environmental Chemistry – Molecular Materials Chemistry –

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Scope of Research

Our research goal is to develop high-performance organic electroluminescence devices, organic solar cells, and polymer materials. Toward this, we carry out syntheses, device fabrications, precise structure characterizations, and quantum chemical calculations for high functional organic materials. Along with exploring novel synthetic routes and novel devices, we perform detailed analyses of structures and dynamics, mainly by sophisticated solid-state NMR spectroscopy, in order to obtain structure–dynamics– property relationships.

KEYWORDS

Organic Light-Emitting Diodes Solid-State NMR Quantum Chemical Calculation Amorphous Materials Dynamic Nuclear Polarization Enhanced NMR



Recent Selected Publications

Shizu, K.; Ren, Y.; Kaji, H., Promoting Reverse Intersystem Crossing in Thermally Activated Delayed Fluorescence via the Heavy-Atom Effect, *J. Phys. Chem. A*, **127**, 439-449 (2023).

Tanaka, H.; Mizuhata, Y.; Tokitoh, N.; Miyamoto, R.; Kanamori, K.; Kaji, H., Multiple Stimuli-Responsive Supramolecular Organic Framework under Concomitant Emission Color Changes, J. Phys. Chem. C, 127, 20459-20465 (2023).

Suzuki, K.; Kaji, H., Torsion Angle Analysis of a Thermally Activated Delayed Fluorescence Emitter in an Amorphous State Using Dynamic Nuclear Polarization Enhanced Solid-State NMR, *J. Am. Chem. Soc.*, **145**, 16324-16329 (2023).

Promoting Reverse Intersystem Crossing in Thermally Activated Delayed Fluorescence via the Heavy-Atom Effect

Fast reverse intersystem crossing (RISC) in thermally activated delayed fluorescence (TADF) is an effective approach to improving the device lifetime of organic light-emitting diodes. In this study, we reported the heavy-atom effect on TADF and a molecular design for accelerating RISC. We reproduced all the relevant rate constants of a sulfur-containing molecule (k_{RISC} of 10⁸ s⁻¹) using density functional theory and revealed the role of the heavy-atom effect on the rapid RISC. Then, we predicted much larger k_{RISC} (>10¹⁰ s⁻¹) for selenium- and telluriumcontaining molecules. We also predicted that a poloniumcontaining molecule would promote phosphorescence without exhibiting TADF, indicating that a too strong heavy-atom effect is disadvantageous for achieving both rapid RISC and efficient TADF. A moderate heavy-atom effect was found to be essential for fast RISC in TADF.

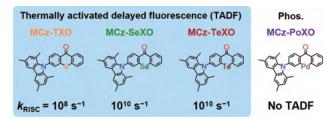


Figure 1. Promoting Reverse Intersystem Crossing in Thermally Activated Delayed Fluorescence.

Torsion Angle Analysis of a Thermally Activated Delayed Fluorescence Emitter in an Amorphous State Using Dynamic Nuclear Polarization Enhanced Solid-State NMR

The torsion angle between donor and acceptor segments of a thermally activated delayed fluorescence (TADF) molecule is one of the most critical factors in determining the performance of TADF-based organic light-emitting diodes (OLEDs) because the torsion angle affects not only the energy gap between the singlet and triplet but also the oscillator strength and spin-orbit coupling. However, the torsion angle is difficult to analyze, because organic molecules are in an amorphous state in OLEDs. Here, we determined the torsion angle of a highly efficient TADF emitter, DACT-II, in an amorphous state by dynamic nuclear polarization-enhanced solid-state NMR measurements. From the experimentally obtained chemical shift principal values of 15N on carbazole, we determined the average torsion angle to be 52°. Such quantification of the torsion angles in TADF molecules in amorphous solids will provide deep insight into the TADF mechanism in amorphous OLEDs.

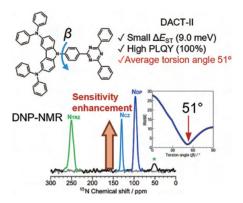


Figure 2. Torsion angle analysis of TADF emitter by DNP-NMR.

Multiple Stimuli-Responsive Supramolecular Organic Framework under Concomitant Emission Color Changes

A stimuli-responsive luminophore embedding an overcrowd-ed bistricyclic aromatic ene structure with a heptagon=hexagon central ring, DCHA-TRZ, has been designed and synthesized. In a single-crystalline solid, DCHA-TRZ constructed a supramolecular organic framework (SOF) including n-hexane molecules as a guest molecule. The crystalline SOF (α phase) exhibited reversible crystalline (α)-to-amorphous-to-crystalline (α) solid-state phase transitions triggered by external stimuli of mechanical grinding and treatment with a *n*-hexane solvent, in which release and inclusion of the guest molecules played an important role. Moreover, the thermal annealing of the amorphous ground solid afforded a bluish green-emitting solid with a different crystalline phase (β). The combination of the three external stimuli of the mechanical grinding, thermal annealing and solvent treatment enables the reversible and cyclical phase transitions among three solidstate phases (crystalline α , β and amorphous) under concomitant emission color changes.



Figure 3. Multiple stimuli-responsive SOF under concomitant emission color changes on the mortar.

Division of Environmental Chemistry – Hydrospheric Environment Analytical Chemistry –

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Institute of Oceanography, National Taiwan University, Taiwan, 27 September 2023–26 October 2023

Scope of Research

(i) Biogeochemistry of trace elements in the hydrosphere: Novel analytical methods are developed for trace metals and their isotopes. Distribution of trace elements in the hydrosphere and their effects on the ecosystem are investigated. The study also covers hydrothermal activity, deep biosphere, and paleocean. (ii) Ion recognition: Novel ligands and ion recognition system are designed, synthesized, and characterized.



KEYWORDS

Marine Chemistry Stable Isotopes Analytical Chemistry Trace Elements Metal Ion Recognition

Recent Selected Publications

Ueki, R.; Zheng, L.; Takano, S.; Sohrin, Y., Distributions of Zirconium, Niobium, Hafnium, and Tantalum in the Subarctic North Pacific Ocean Revisited with a Refined Analytical Method, *Geochem J.*, **57**, 143-154 (2023).

Matsuoka, K.; Tatsuyama, T.; Takano, S.; Sohrin, Y., Distribution of Stable Isotopes of Mo and W from a River to the Ocean: Signatures of Anthropogenic Pollution, *Front. Mar. Sci.*, **10** (2023).

Sieber, M.; Lanning, N. T.; Bian, X.; Yang, S.-C.; Takano, S.; Sohrin, Y.; Weber, T. S.; Fitzsimmons, J. N.; John, S. G.; Conway, T. M., The Importance of Reversible Scavenging for the Marine Zn Cycle Evidenced by the Distribution of Zinc and Its Isotopes in the Pacific Ocean, *J. Geophys. Res.: Oceans*, **128** (2023).

Alam, M.; Muguli, T.; Gurumurthy, G. P.; Arif, M.; Sohrin, Y.; Singh, A. D.; Radhakrishna, T.; Pandey, D. K.; Verma, K., Hydroclimatic Conditions and Sediment Provenance in the Northeastern Arabian Sea since the Late Miocene: Insights from Geochemical and Environmental Magnetic Records at IODP Site U1457 of the Laxmi Basin, *Geol Mag.*, **160**, 813-829 (2023).

Iwase, M.; Isobe, K.; Zheng, L.; Takano, S.; Sohrin, Y., Solid-Phase Extraction of Palladium, Platinum, and Gold from Water Samples: Comparison between a Chelating Resin and a Chelating Fiber with Ethylenediamine Groups, *Anal. Sci*, **39**, 695-704 (2023).

Distribution of Stable Isotopes of Mo and W from a River to the Ocean: Signatures of Anthropogenic Pollution

Molybdenum (Mo) and tungsten (W) are redox-sensitive elements, and their stable isotope ratios have attracted attention as paleoceanographic proxies. However, our knowledge of the distribution of stable Mo and W isotopes in the modern hydrosphere remains limited. In this study, we provided the concentrations and isotope ratios of dissolved Mo and W in the oceans (the North Pacific and Indian Oceans), marginal seas (East China and the Sea of Japan), and a river-estuary system in Japan (from the Uji-Yodo rivers to Osaka Bay). In the North Pacific and Indian Oceans, the W concentration was 48.2 ± 6.2 pmol/ kg (ave ± 2 sd, n = 109), $\delta^{186/184}$ W was 0.52 ± 0.06 ‰, the Mo concentration was 105.1 ± 8.0 nmol/kg, and $\delta^{98/95}$ Mo was 2.40 ± 0.06 %. The results indicate that W has the constant concentration and isotopic composition in the modern ocean as well as Mo. In the East China Sea and the Sea of Japan, the W concentration and $\delta^{186/184}$ W in the upper water (< 1000 m depth) were different from those in the ocean (W = 56 \pm 18 pmol/kg, $\delta^{186/184}W$ = 0.45 \pm 0.06 ∞ , n = 24). However, the concentrations in deeper water were congruent with those in the oceans (W = 49.9 ± 7.6 pmol/kg, $\delta^{186/184}$ W = 0.50 ± 0.02 ‰, *n* = 7). The Mo concentration was 105.4 \pm 3.1 nmol/kg and $\delta^{98/95}Mo$ was 2.36 $\pm 0.03 \% (n = 31)$ throughout the water column, congruent with those in the ocean. In the Uji River-Yodo River-Osaka Bay system, the W concentration reached 1074 pmol/kg and $\delta^{186/184}$ W reached 0.20 ‰. We propose that the enrichment of W with a low $\delta^{186/184}$ W in the river-estuary system and marginal seas is caused by anthropogenic pollution. Anthropogenic Mo pollution was not detected in marginal seas. However, the Mo concentration and $\delta^{98/95}$ Mo showed high anomalies above the mixing line of river water and seawater in the lower Yodo River and Osaka Bay, implying possible anthropogenic pollution of Mo in the metropolitan area.

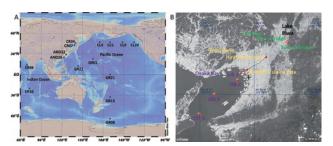


Figure 1. Sampling stations of this study: A, global map; B, map of the Uji River-Yodo River-Osaka Bay system.

Distributions of Zirconium, Niobium, Hafnium, and Tantalum in the Subarctic North Pacific Ocean Revisited with a Refined Analytical Method

Although zirconium (Zr), niobium (Nb), hafnium (Hf), and tantalum (Ta) in seawater are potential tracers for water masses, their determination is still a challenge in analytical chemistry. We have refined our preconcentration method using 8-hydroxyquinoline chelating resin (TSK-8HQ) and reinvestigated concentration profiles of the four elements in dissolved (d) and total dissolvable (td) fractions at five different stations from 47 °N, 160 °E to 51 °N, 160 °W in the subarctic North Pacific Ocean. The new method has saved analytical time and reduced systematic errors compared with previous methods. The concentration ranges were 30 - 276 pmol/kg for dZr, 1.0 - 2.6 pmol/kg for dNb, 0.09 - 0.78 pmol/kg for dHf, and 0.006 - 0.026 pmol/kg for dTa in the subarctic North Pacific Ocean. The concentrations of Zr and Hf increased from surface water to deep water, whereas those of Nb and Ta were nearly constant over the water depth. The profiles of dZr, dNb, and dHf were consistent with those in previous studies. However, we found that dTa is uniformly distributed at 0.015 ± 0.005 pmol/kg (mean \pm sd, n = 75), which is approximately onefifth of that in a previous study. It is likely that the previous dTa data were affected by a systematic error. Negligible differences between td and d fractions suggest that the particulate concentrations of these elements are lower than those reported in a previous study.

Comparison of dissolved Ta at crossover stations

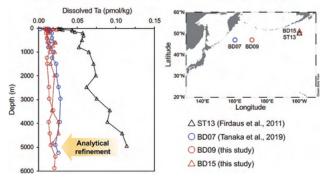


Figure 2. Graphical abstract of this study.

Division of Environmental Chemistry – Chemistry for Functionalized Surfaces –

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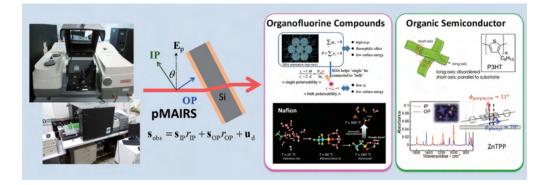
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Scope of Research

To understand the chemical structure and properties of a molecular aggregated system, the keywords of molecular interactions and orientation are focused on, and the molecular aggregates are investigated by using originally developed spectroscopic techniques. The current major topics are: (1) perfluoroalkyl-specific properties in a condensed system; (2) controlling factors of molecular packing and orientation in a thin film of an organic semiconductor compound; (3) development of new molecular orientation analytical technique "MAIRS2."

KEYWORDS

Infrared and Raman Spectroscopy Surface and Interface Chemistry Perfluoroalkyl Compounds Organic Semiconductors pMAIRS and MAIRS2



Recent Selected Publications

Shimoaka, T.; Yamaguchi, Y.; Shioya, N.; Ajayaghosh, A.; Mori, T.; Ariga, K.; Hasegawa, T., Insights on the Molecular Orientation of Oligo(*p*-Phenylene Vinylene) Derivatives with Alkyl Chains in Langmuir Films, *J. Phys. Chem. C.*, **127**, 9336-9343 (2023).

Oka, T.; Shioya, N.; Shimoaka, T.; Hasegawa, T., Structural Rearrangement of Organic Semiconductor Molecules with an Asymmetric Shape in Thin Films, *J. Phys. Chem. C.*, **127**, 7560-7564 (2023).

Shioya, N.; Yoshida, M.; Fujii, M.; Shimoaka, T.; Miura, R.; Maruyama, S.; Hasegawa, T., Conformational Change of Alkyl Chains at Phase Transitions in Thin Films of an Asymmetric Benzothienothiophene Derivative, *J. Phys. Chem. Lett.*, **13**, 11918-11924 (2022).

Shioya N.; Fujii M.; Shimoaka T.; Eda K.; Hasegawa T., Stereoisomer-Dependent Conversion of Dinaphthothienothiophene Precursor Films, *Sci. Rep.*, **12**, 4448 (2022).

Tomita K.; Shioya N.; Shimoaka T.; Wakioka M.; Hasegawa T., Control of Supramolecular Organizations by Coordination Bonding in Tetrapyridylporphyrin Thin Films, *Chem. Commun.*, **58**, 2116-2119 (2022).

Insights on the Molecular Orientation of Oligo(*p*-Phenylene Vinylene) Derivatives with Alkyl Chains in Langmuir Films

One of the oligo(p-Phenylene Vinylene) derivatives having alkyl chains, OPV-1, is known to form rod-shaped nanoaggregates on the water surface, and thin films with aligned nanoaggregates can be obtained by the Langmuir-Blodgett (LB) technique. Although the molecular aggregation and orientation of the "conjugated rings part" in the LB films have already been investigated, analysis of the detailed molecular structure involving the "alkyl chains" is left behind. In the present study, to reveal the role of the alkyl chains in the molecular aggregation in Langmuir films prior to the LB transfer, infrared (IR) external reflection spectroscopic measurements on the water surface are carried out. It has been revealed that not only the conjugated rings of OPV-1 but also the alkyl chains with an ordered conformation are lying on the water surface. In addition, the orientation is found to be kept on a solid substrate even after the LB transfer by IR p-polarized multiple-angle incidence resolution spectrometry.

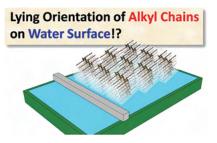


Figure 1. Lying orientation of oligo(*p*-phenylene vinylene) derivatives on the water surface.

Structural Rearrangement of Organic Semiconductor Molecules with an Asymmetric Shape in Thin Films

2-Decyl-7-phenyl[1]benzothieno[3,2-b][1]benzothiophene (Ph-BTBT-C10) exhibits excellent performances as an active layer in organic thin-film transistors, and its performances are greatly influenced by the molecular packing, i.e., the crystalline polymorphs. This compound has the so-called thin-film phase in a vapor-deposited film, which is different from the single-crystal structure (the bulk phase). In this work, thin films of Ph-BTBT-C10 are prepared by spin coating, and the effect of aging on the film structure is investigated by high-resolution IR spectroscopy in combination with X-ray diffraction. The results show that the as-spun film has the same thin-film phase as the vapordeposited film and that the thin-film phase is rapidly converted to the bulk phase by aging at room temperature. This work highlights the importance of using IR spectroscopy with a high-wavenumber resolution for structural analysis of molecular thin films.

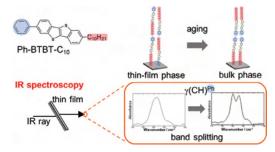


Figure 2. Structural rearrangement of Ph-BTBT-C10 from the thin-film phase to the bulk phase revealed by IR spectroscopy.

Conformational Change of Alkyl Chains at Phase Transitions in Thin Films of an Asymmetric Benzothienobenzothiophene Derivative

Ph-BTBT-C10 has a highly ordered liquid crystalline state, i.e., the smectic E (SmE) phase. Although the transition from the crystalline state to the SmE phase is believed to accompany melting of the alkyl chains, no spectroscopic evidence has been found so far. In this study, the conformational change of the decyl chains in Ph-BTBT-C10 films across the phase transition is analyzed by temperaturedependent measurements in situ using IR spectroscopy. The spectral analysis reveals that the polycrystalline film has latent conformational disorder (the gauche conformer), the rate of which becomes more pronounced with the heat treatment. As expected, melting of the decyl chains is observed above the transition temperature to the SmE phase.

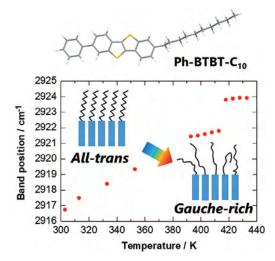


Figure 3. Conformational change of alkyl chains of Ph-BTBT-C10 with temperature.

Division of Environmental Chemistry – Molecular Microbial Science –

https://www.scl.kyoto-u.ac.jp/~mmsicr/mmstojp/Top_en.html



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Scope of Research

Microorganisms are found almost everywhere on Earth. They have a great diversity of capacities to adapt to various environments, including chemically and physically unusual environments. Our main subject is to clarify the molecular basis of environmental adaptations of microorganisms and their application. Specific functions of proteins and lipids with essential roles in environmental adaptation of extremophilic microorganisms are of our particular interest. We also undertake mechanistic analysis of microbial enzymes, in particular, those involved in unique metabolic pathways, and their application.



KEYWORDS

Extremophiles Phospholipid Acyltransferase Bacterial Cold-Adaptaion Mechanism Extracellular Membrane Vesicle Polyunsaturated Fatty Acid

Recent Selected Publications

Kawano, K.; Kamasaka, K.; Yokoyama, F.; Kawamoto, J.; Ogawa, T.; Kurihara, T.; Matsuzaki K., Structural Factors Governing Binding of Curvature-Sensing Peptides to Bacterial Extracellular Vesicles Covered with Hydrophilic Polysaccharide Chains, *Biophys. Chem.*, **299**, 107039 (2023).

Kamasaka, K.; Kawamoto, J.; Tsudzuki, T.; Liu, Y.; Imai, T.; Ogawa, T.; Kurihara, T., Capsular Polysaccharide-Mediated Protein Loading onto Extracellular Membrane Vesicles of a Fish Intestinal Bacterium, *Shewanella vesiculosa* HM13, *bioRxiv*, 04.25.538355 (2023).

Mullane, K. K.; Nishiyama, M.; Kurihara, T.; Bartlett, D. H., Compounding Deep Sea Physical Impacts on Marine Microbial Motility, *Front. Mar. Sci.*, **10** (2023).

Ogawa, T.; Kuboshima, M.; Suwanawat, N.; Kawamoto, J.; Kurihara, T., Division of the Role and Physiological Impact of Multiple Lysophosphatidic Acid Acyltransferase Paralogs, *BMC Microbiol.*, **1**, 241 (2022).

Conversion of Docosahexaenoic Acid to Eicosapentaenoic Acid by β-Oxidation Enzymes in *Shewanella livingstonensis* Ac10

Shewanella livingstonensis Ac10, a cold-adapted Gramnegative bacterium isolated from Antarctic seawater, produces eicosapentaenoic acid (EPA) at low temperatures. An EPA-less mutant strain (Δ EPA) showed delayed growth and cold-sensitive phenotypes. Δ EPA cultured in the medium supplemented with docosahexaenoic acid (DHA)-containing phospholipids grew normally at low temperatures. Interestingly, the mutant contained not only DHA-containing phospholipids but also EPA-containing phospholipids even though it cannot produce EPA de novo. These results suggested S. livingstonensis Ac10 requires EPA or DHA to adapt to low temperatures, and it has an unknown conversion pathway of DHA to EPA to generate EPA selectively. Previous studies demonstrated that first two β -oxidation enzymes, acyl-CoA dehydrogenase (FadE) and 2,4-dienoyl-CoA reductase (FadH), are involved in this conversion of DHA to EPA. Therefore, the conversion pathway is likely identical or similar to the β -oxidation pathway. On the other hand, it is unclear how EPA is produced from DHA by β -oxidation, in which a series of oxidation reactions repeatedly occur to degrade fatty acids into acetyl-CoA in general, and whether the last two βoxidation enzymes, FadB and FadA, or FadJ and FadI, are involved in this conversion. Gene-deletion analysis of these genes demonstrated that, in the single fad mutant strains, EPA converted from DHA was accumulated, and EPA-containing phospholipids were produced. $\Delta EPA/$ Δ FadJ had DHA more than the others, and unknown fatty acids predicted as intermediates were observed in the mutant. However, every fad mutant, including $\Delta EPA/\Delta FadJ$, still has the conversion ability, indicating the redundant role of FadB/FadJ and FadA/FadI in the conversion. Therefore, double knockout strains, $\Delta EPA/\Delta FadBJ$ and $\Delta EPA/\Delta FadBJ$ Δ FadAI, were constructed. In Δ EPA/ Δ FadBJ strain, the DHA-to-EPA conversion rate was decreased by 32% compared with ΔEPA . These results revealed the β oxidation enzymes play a role in the DHA-EPA conversion of this bacterium.

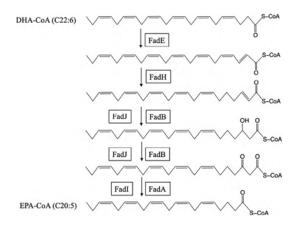


Figure 1. Putative conversion pathway of DHA to EPA.

Screening and Identification of Genes Involved in Extracellular Membrane Vesicle Production of *Shewanella vesiculosa* HM13

Extracellular membrane vesicles (EMVs) are lipid nanoparticles secreted by almost all bacteria, and their physiology and biotechnological applications have been attracting significant attention. However, the molecular basis of EMV biogenesis has yet to be fully elucidated. To facilitate the elucidation of bacterial EMV production, a curvature-sensing peptide, nFAAV5-NBD, was developed by using a hyper-vesiculating bacterium, Shewanella vesiculosa HM13, as a model organism. nFAAV5-NBD can bind to EMVs of this bacterium but not to the cells. In this study, we applied nFAAV5-NBD to screen a hypervesiculation and hypo-vesiculation mutant from the mutant library generated by transposon random mutagenesis (Fig. 2). As a result, we identified 16 or six genes whose transposon insertions caused hyper- or hypo-vesiculation, respectively. Identification of the transposon-insertion site indicated that genes involved in various cell processes, including protein quality control, cell wall synthesis, and signal transduction, are involved in the EMV production of S. vesiculosa HM13. A target gene disruption analysis of the identified genes also demonstrated the changes in EMV production of the mutants. These strains obtained in this study would contribute to the elucidation of bacterial vesicle formation mechanisms. Additionally, the hyper-vesiculating mutants obtained from this study would provide a clue for the application of this bacterium, for example, the production of valuable substances as a cargo of EMVs and the development of surface-engineered vesicles.

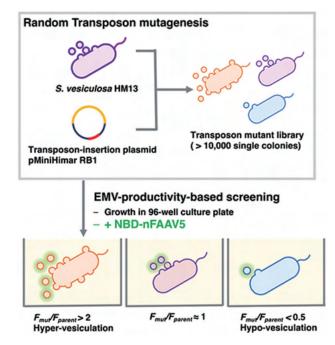


Figure 2. Schematic illustration of the high-throughput screening of the mutants with changes in EMV production of *S. vesiculosa* HM13.

Division of Multidisciplinary Chemistry – Polymer Materials Science –

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Scope of Research

The structure and molecular motion of polymer substances are studied, mainly using scattering methods such as X-ray, neutron, and light with intent to solve fundamentally important problems in polymer science. The main projects are studied on 1) the morphologies and the dynamics of self-assembling processes in block copolymers, 2) the hierarchical structures in crystalline polymer and rubber-filler systems, 3) the viscoelastic effects in glassy materials, 4) formation processes and ordering structures in polymer thin films.

KEYWORDS

Polymer Physics Self Assembly Hierarchical Structure Polymer Properties Softmatter



Recent Selected Publications

Nakanishi, Y.; Ishige, R.; Ogawa, H.; Huang, Y.; Sakakibara, K.; Ohno, K.; Kanaya, T.; Takenaka, M.; Tsujii, Y., Unified Explanation for Self-Assembly of Polymer-Brush-Modified Nanoparticles in Ionic Liquids, *Polym. J.*, 55, 1199-1209 (2023).

Shibata, M.; Nakanishi, Y.; Abe, J.; Arima-Osonoi, H.; Iwase, H.; Shibayama, M.; Motokawa, R.; Kumada, T.; Takata, S.; Yamamoto, K.; Takenaka, M.; Miyazaki, T., Structural Changes of Polystyrene Particles in Subcritical and Supercritical Water Revealed by in situ Small-Angle Neutron Scattering, *Polym. J.*, **55**, 1165-1170 (2023).

Watanabe, Y.; Ogawa, H.; Konishi, T.; Nishitsuji, S.; Ono, S.; Shimizu, N.; Takenaka, M., Distribution of Oriented Lamellar Structures in Injection-Molded High-Density Polyethylene Visualized via the Small Angle X-ray Scattering-Computed Tomography Method, *Macromolecules*, **56(15)**, 5964-5973 (2023).

Watanabe, Y.; Nishitsuji, S.; Takenaka, M., Anomalous Small-Angle X-ray Scattering Analyses on Hierarchical Structures of Rubber–Filler Systems, J. Appl. Crystallogr., 56 (2), 461-467 (2023).

Kishimoto, M.; Takenaka, M.; Iwabuki, H., Spatial Distribution of the Amorphous Region Constrained by Polymer Crystallites, *Macromolecules*, **56** (1), 207-214 (2023).

Anomalous Small-Angle X-Ray Scattering Analyses on Hierarchical Structures of Rubber–Filler Systems

The hierarchical structures of carbon black (CB) in Poly(styrene-ran-butadiene) (SBR) rubber/CB systems vulcanized with sulfur and ZnO were clarified by using anomalous small-angle X-ray scattering (ASAXS) near the Zn absorption edge. The SBR/CB systems vulcanized with sulfur and ZnO are commonly used and quantitative analyses of the hierarchical structures in the SBR/CB systems are needed. However, the hierarchical structures in the SBR/CB systems have not been well investigated since the strong scattering contrast of Zn hinders the quantitative analyses of the hierarchical structures of CB by using X-ray scattering. In this study, we eliminated the effects of Zn on the scattering intensity and obtained the structure factors of CB in SBR/CB systems by using the ASAXS method. By extrapolating the structure factors of CB to a zero-volume fraction of CB, we were able to estimate the particle structure factor of the CB aggregate and found that the CB aggregates consist of the closely-packed CB primary particles. We also found the existence of the large particles of ZnO and the particles of ZnS in the order of 10 nm in the structure factors of Zn.

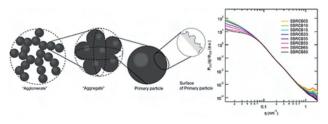


Figure 1. Schematic for hierarchical structures of filler in rubber. Partial scattering function $P_{\rm CC}(q)/\phi_{\rm CB}$ of CB for all samples.

Distribution of Oriented Lamellar Structures in Injection-Molded High-Density Polyethylene Visualized via SAXS-CT Method

We successfully reconstructed the spatial distribution of the orientation of the lamellar structures in injectionmolded high-density polyethylene (HDPE) using the small-angle X-ray scattering-computed tomography (SAXS-CT) technique, a combination of the SAXS and CT methods. The skin, subskin, and core layers were identified in the obtained images of the distribution. The orientation and thickness in each layer were found to vary with the injection speed, v. At the slowest v of 5 mm/s, a skin layer is formed along the surface of the sample with the lamellar structure oriented in the injection direction. At the center of the sample, the orientation of the lamellar structure is isotropic, i.e., the core layer. Between the skin and core layers, there is the subskin layer where the lamellar structures are oriented perpendicular and parallel to the injection direction. The thickness of the core layer decreases for $5 \leq$ $v \le 20$ mm/s because the higher elongation of the polymer chains due to the shear deformation is dominant. For $20 \le$ $v \le 40$ mm/s, the strength of the fountain flow and the shear deformation affect the thickness of the layers. The core layer corresponds to the outlet portion of the fountain flow. The increase in the fountain flow amount inhibits the higher orientation of polymer chains, resulting in an almost constant thickness of the core layer with v. In the subskin layer, the increase in the higher elongation of polymer chains with *v* induces an increase in the thickness for $5 \le v$ ≤ 20 mm/s. Although the velocity gradient is even more significant, the suppression of the polymer chain orientation by the fountain flow can result in a nearly constant subskin layer thickness for $20 \le v \le 40$ mm/s. The flux of polymers originating from the fountain flow oriented perpendicular to the injection direction is dominant. Unlike the exponential changes in the core and subskin layers, the thickness of the skin layer decreases in proportion to the increase in v potentially because the fountain flow effect increases for $5 \le v \le 40$ mm/s, suppressing the shear deformation near the mold.

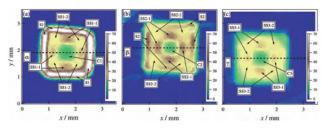


Figure 2. SAXS-CT images in the X-Y plane reconstructed from the SAXS profiles at each φ_1 and Y. Each injection speed condition is v = 5 mm/s for (a), 20 mm/s for (b), and 40 mm/s for (c). The injection direction is toward the front of the paper.

Division of Multidisciplinary Chemistry – Molecular Rheology –

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Scope of Research

Research focus is placed on the molecular origin of rheological properties of various materials. Depending on time and temperature, homogeneous polymeric materials exhibit typical features of glass, rubber, and viscous fluid while heterogeneous polymeric systems exhibit plasticity in addition to these features. For basic understanding of these features, the molecular motion and structures at various scales are studied for polymeric systems in deformed state. Rheological measurements are performed with various rheometers. Auto-correlation of the molecular orientation is also investigated with dynamic dielectric spectroscopy. Analysis of rheological and dielectric behavior elucidates a new aspect of softmatter physics.

Assist Prof

SATO, Takeshi

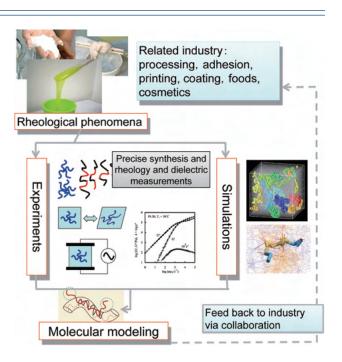
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KEYWORDS

Rheology	Dielectric Spectroscopy
Soft Matter	Mesoscopic Model



Recent Selected Publications

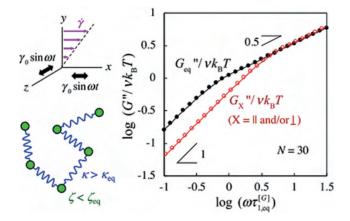
Sato, T.; Gong, Y.; Larson, R. G., Testing the Ability of the Slip-Spring Model to Describe Constraint Release Effects Using Experimental Linear and Nonlinear Rheology, *Macromolecules*, **56**, 8116-8132 (2023).

Miyamoto, S.; Sato, T.; Taniguchi, T., Stretch-Orientation-Induced Reduction of Friction in Well-Entangled Bidisperse Blends: a Dual Slip-Link Simulation Study, *Rheologica Acta*, **62**, 57-70 (2023).

Matsumiya, Y.; Sato, T.; Chen, Q.; Watanabe, H., Rouse Analysis of Nonlinear Rheology of Unentangled Polymer Melts under Fast Shear: Viscoelastic Response to Superposed Oscillatory Strain, *Macromolecules*, **56**, 2930-2983 (2023).

Rouse Analysis of Nonlinear Rheology of Unentangled Polymer Melts under Fast Shear: Viscoelastic Response to Superposed Oscillatory Strain

Nonlinear rheological behavior of unentangled polymer melts can be described by the Rouse model given that its parameters, spring strength κ , bead friction coefficient ζ , and mean-square Brownian force intensity B, are allowed to change under fast flow/large strain (and to take anisotropic tensorial forms when necessary). Within this model, analytic expressions in terms of those parameters have been obtained for measurable quantities that include viscosity η , the first normal stress difference coefficient Ψ_1 , and complex dielectric permittivity ɛ*. Those expressions in turn enable us to extract κ , ζ , and B from experimental data of unentangled melts. In particular, the rheo-dielectric ε^* data under shear, recently obtained for unentangled low-M poly (butylene oxide) melt having type-A dipoles (PBO-16k; $M = 16 \times 10^3$), suggest that the tensorial ζ and B have negligibly small off-diagonal components in a range of Weissenberg number Wi up to 1.2. On the basis of that study, we here focus on the complex shear moduli G_{\parallel}^* and G_{\perp}^{*} of the Rouse chain defined as responses to a small oscillatory strain superposed on the steady shear flow, with \parallel and \perp representing parallel and perpendicular superposition, respectively. In the case of negligible off-diagonal components of ζ and B, the Rouse analysis gave a very simple expression of those moduli, $G_X^*(\omega) = b_X^{[G]} G_{eq}^*(\omega \alpha_X^{[G]})$ with $X = \parallel$ and \perp , where $G_{eq}^*(\omega)$ is the linear viscoelastic (LVE) complex modulus at an angular frequency ω . Namely, in that case, the relaxation time of G_X^* decreases by a factor of $\alpha_X^{[G]}$ (<1) and its terminal relaxation intensity is enhanced by a factor of $b_{\chi}^{[G]}(>1)$, but a relative distribution of the relaxation modes exhibits no change. Furthermore, the Rouse parameters obtained from the η , Ψ_1 , and ϵ^* data of PBO-16k were found to satisfy a specific empirical relationship, $\{b_{\parallel}^{[G]}\}^2 \cong 1/\alpha_{\parallel}^{[G]}$. Because $G'_{eq}(\omega) \cong G''_{eq}(\omega) \propto \omega^{1/2}$ at high ω where the LVE Rouse relaxation has not completed, this relationship suggests $G''_{\parallel}(\omega) = G''_{eq}(\omega)$ at $\omega > 1/\tau^{[G]}_{\parallel}$ and $G''_{\parallel}(\omega) \leq G''_{eq}(\omega)$ at $\omega \leq 1/\tau_{\parallel}^{[G]}$, where $\tau_{\parallel}^{[G]}$ is the terminal viscoelastic relaxation time defined for $G_{\parallel}^{*}(\omega)$. This behavior of $G''_{\parallel}(\omega)$ is superficially equivalent to that expected for a case of disappearance of viscous contributions of low-order Rouse eigenmodes under fast shear discussed in the literature on the basis of the concept of Pincus blob. However, the current Rouse analysis clearly indicated that all eigenmodes keep their viscous contributions with a magnitude determined by ζ and κ under flow, confirming the importance of nonequilibrium changes of ζ and κ in the nonlinear flow behavior of unentangled melts.



Division of Multidisciplinary Chemistry - Molecular Aggregates -

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Scope of Research

We design and synthesize unique electronic materials with sophisticated device applications in mind. These materials have novel solid-state aggregation structures or well-defined interface orientation that promote efficient electrical current flow or enhance device lifetime. Electronic devices based on these new materials are then evaluated using advanced measurement techniques, and the results are used to inform the next direction of the materials chemistry. We call this synergistic approach for achieving our research goals "Needs Inspired Fundamental Science".



KEYWORDS

Molecular Design and Synthesis

Molecular Aggregation **Functional Materials** Semiconductors Perovskite Solar Cells

Recent Selected Publications

Hu, S.; Zhao, P.; Nakano, K.; Oliver, R. D. J.; Pascual, J.; Smith, J. A.; Yamada, T.; Truong, M. A.; Murdey, R.; Shioya, N.; Hasegawa, T.; Ehara, M.; Johnston, M. B.; Tajima, K.; Kanemitsu, Y.; Snaith, H. J.; Wakamiya, A., Synergistic Surface Modification of Tin-Lead Perovskite Solar Cells, Adv. Mater., 35, 2208320 (2023).

Truong, M. A.; Funasaki, T.; Ueberricke, L.; Nojo, W.; Murdey, R.; Yamada, T.; Hu, S.; Akatsuka, A.; Sekiguchi, N.; Hira, S.; Xie, L.; Nakamura, T.; Shioya, N.; Kan, D.; Tsuji, Y.; Iikubo, S.; Yoshida, H.; Shimakawa, Y.; Hasegawa, T.; Kanemitsu, Y.; Suzuki, T.; Wakamiya, A., Tripodal Triazatruxene Derivative as a Face-On Oriented Hole-Collecting Monolayer for Efficient and Stable Inverted Perovskite Solar Cells, J. Am. Chem. Soc., 145, 7528-7539 (2023).

Tan, T.; Nakamura, T.; Murdey, R.; Hu, S.; Truong, M. A.; Wakamiya, A., BAr₂-Bridged Azafulvene Dimers with Tunable Energy Levels for Photostable Near-Infrared Dyes, Chem. Eur. J., 29, e202300529 (2023).

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Liu, W.; Hu, S.; Pascual, J.; Nakano, K.; Murdey, R.; Tajima, K.; Wakamiya, A., Tin Halide Perovskite Solar Cells with Open-Circuit Voltages Approaching the Shockley-Queisser Limit, ACS Appl. Mater. Interfaces, 15, 32487-32495 (2023).

Synergistic Surface Modification of Tin–Lead Perovskite Solar Cells

Interfaces in thin-film photovoltaics play a pivotal role in determining device efficiency and longevity. In this work, the top surface treatment of mixed tin-lead (≈1.26 eV) halide perovskite films for p-i-n solar cells is studied. Charge extraction is promoted by treating the perovskite surface with piperazine. This compound reacts with the organic cations at the perovskite surface, modifying the surface structure and tuning the interfacial energy level alignment. In addition, the combined treatment with C₆₀ pyrrolidine tris-acid (CPTA) reduces hysteresis and leads to efficiencies up to 22.7%, with open-circuit voltage values reaching 0.90 V, \approx 92% of the radiative limit for the bandgap of this material. The modified cells also show superior stability, with unencapsulated cells retaining 96% of their initial efficiency after >2000 h of storage in N₂ and encapsulated cells retaining 90% efficiency after >450 h of storage in air. Intriguingly, CPTA preferentially binds to Sn²⁺ sites at film surface over Pb²⁺ due to the energetically favored exposure of the former, according to first-principles calculations. This work provides new insights into the surface chemistry of perovskite films in terms of their structural, electronic, and defect characteristics and this knowledge is used to fabricate state-of-the-art solar cells.1)



Figure 1. Surface modification of tin–lead perovskite films with piperazine and CPTA.

Tripodal Triazatruxene Derivative as a Face-On Oriented Hole-Collecting Monolayer for Efficient and Stable Inverted Perovskite Solar Cells

Hole-collecting monolayers have drawn attention in perovskite solar cell research due to their ease of processing, high performance, and good durability. Since molecules in the hole-collecting monolayer are typically composed of functionalized π -conjugated structures, hole extraction is expected to be more efficient when the π -cores are oriented face-on with respect to the adjacent surfaces. However, strategies for reliably controlling the molecular orientation in monolayers remain elusive. In this work, multiple phosphonic acid anchoring groups were used to control the molecular orientation of a series of triazatruxene derivatives chemisorbed on a transparent conducting oxide electrode surface. Using infrared reflection absorption spectroscopy and metastable atom electron spectroscopy, we found that multipodal derivatives align face-on to the electrode surface, while the monopodal counterpart adopts a more tilted configuration. The face-on orientation was found to facilitate hole extraction, leading to inverted perovskite solar cells with enhanced stability and high-power conversion efficiencies up to 23.0%.²⁾

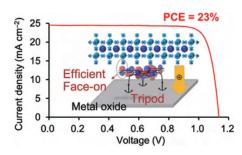
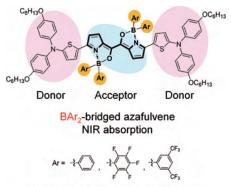


Figure 2. Triazatruxene-based tripodal hole collecting monolayer for inverted perovskite solar cells.

BAr₂-Bridged Azafulvene Dimers with Tunable Energy Levels for Photostable Near-Infrared Dyes

Organic dyes with strong absorption in the near-infrared (NIR) region are potentially useful in medical applications, such as tumor imaging and photothermal therapy. In this work, new NIR dyes combining BAr₂-bridged azafulvene dimer acceptors with diarylaminothienyl donors in a donor–acceptor–donor configuration were synthesized. Surprisingly, it was found that in these molecules the BAr₂-bridged azafulvene acceptor adopts a 5-membered, rather than 6-membered ring structure. The influence of the aryl substituents on the HOMO and LUMO energy levels of the dye compounds was assessed from electrochemical and optical measurements. Strong electron-withdrawing fluorinated substituents (Ar = C_6F_5 , 3,5-(CF_3)₂ C_6H_3) lowered the HOMO energy while preserving the small HOMO–LUMO energy gap, resulting in promising NIR dye molecules that combine strong absorption bands centered around 900 nm with good photostability.³)



Tuning the energy levels by Ar groups

Figure 3. BAr₂-bridged azafulvene dimer for photostable near-infrared dyes.

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S. Hu, P. Zhao, K. Nakano, R. D. J. Oliver, J. Pascual, J. A. Smith, T. Yamada, M. A. Truong, R. Murdey, N. Shioya, T. Hasegawa, M. Ehara, M. B. Johnston, K. Tajima, Y. Kanemitsu, H. J. Snaith, A. Wakamiya, *Adv. Mater.*, **35**, 2208320 (2023).

M. A. Truong, T. Funasaki, L. Ueberricke, W. Nojo, R. Murdey, T. Yamada, S. Hu, A. Akatsuka, N. Sekiguchi, S. Hira, L. Xie, T. Nakamura, N. Shioya, D. Kan, Y. Tsuji, S. Iikubo, H. Yoshida, Y. Shimakawa, T. Hasegawa, Y. Kanemitsu, T. Suzuki, A. Wakamiya, *J. Am. Chem. Soc.*, 145, 7528-7539 (2023).

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Advanced Research Center for Beam Science - Particle Beam Science -

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*New Research Field Development Project

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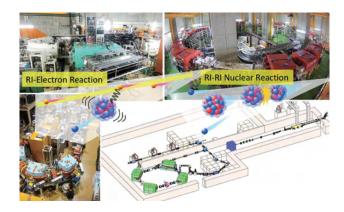
Scope of Research

One of our research is an experimental research for unstable nuclear structures by means of the electron and heavy-ion accelerators. We address the technical development in an RI beam production driven by a high-energy electron beam, an electron scattering from the RI's in combination with the RI target inserted in an electron storage ring, and the precision mass measurement for extremely short-lived and rare exotic nuclei using a heavy-ion storage ring. We will address some technical development aiming at a nuclear photo-absorption cross-section measurement and the beam recycling in a heavy-ion storage ring to study the nuclear reactions involving rare exotic nuclei.

KEYWORDS

Beam Physics Unstable Nuclear Physics Electron Linac

Accelerator Physics Storage Ring



Recent Selected Publications

Tsukada, K.; Abe, Y.; Enokizono, A.; Goke, T.; Hara, M.; Honda, Y.; Hori, T.; Ichikawa, S.; Ito, Y.; Kurita, K.; Legris, C.; Maehara, Y.; Ohnishi, T.; Ogawara, R.; Suda, T.; Tamae, T.; Wakasugi, M.; Watanabe, M.; Wauke, H., First Observation of Electron Scattering from Online-Produced Radioactive Target, Phys. Rev. Lett., 131, 092502 (2023).

Ogawara, R.; Abe, Y.; Ohnishi, T.; Enokizono, A.; Hara, M.; Hori, T.; Ichikawa, S.; Kurita, K.; Maehara, Y.; Suda, T.; Tsukada, K.; Wakasugi, M.; Watanabe, M.; Wauke, H., Ion-Trapping Properties of SCRIT: Time Evolutions of 138Ba Charge State Distributions, Nucl. Instr. Met., B541, 90-92 (2023).

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Li, H. F.; Naimi, S.; Sprouse, T. M.; Mumpower, M. R.; Abe, Y.; Yamaguchi, Y.; Nagae, D.; Suzaki, F.; Wakasugi, M.; Arakawa, H.; Dou, W. B.; Hamakawa, D.; Hosoi, S.; Inada, Y.; Kajiki, D.; Kobayashi, T.; Sakaue, M.; Yokoda, Y.; Yamaguchi, T.; Kagesawa, R.; Kamioka, D.; Moriguchi, T.; Mukai, M.; Ozawa, A.; Ota, S.; Kitamura, N.; Masuoka, S.; Michimasa, S.; Baba, H.; Fukuda, N.; Shimizu, Y.; Suzuki, H.; Takeda, H.; Ahn, D. S.; Wang, M.; Fu, C. Y.; Wang, Q.; Suzuki, S.; Ge, Z.; Litvinov, Yu. A.; Lorusso, G.; Walker, P. M.; Podolyak, Zs.; Uesaka, T., First Application of Mass Measurements with the Rare-RI Ring Reveals the Solar r-Process Abundance Trend at A = 122 and A = 123, Phys. Rev. Lett., 128, 152701 (2022).

Kusumoto, T.; Inoue, S.; Ogawara, R.; Kodaira, S., Measurement of the Energy Spectrum of Laser-Accelerated Protons Using FNTD: Development of an Easy and Quick Method for Energy Spectrometry, Radiat. Meas., 151, 106715 (2022).

Electron Scattering for Determining Charge Density Distribution of Unstable Nuclei

As demonstrated in the 1950s by Hofstadter and his colleagues, high-energy electron scattering is one of the most powerful and reliable methods to reveal the internal structure of atomic nuclei. This is because of the following features: 1) an electron is an elementary particle and has no internal structure, 2) the electro-magnetic interaction is well understood and there is almost no ambiguity in theoretical calculations, and 3) electrons can probe deep inside the nucleus without causing any serious disturbance. In the latter half of the 20th century, many nuclei were investigated by electron scattering, and numerous basic and important features of nuclei, especially stable nuclei, were established.

After progresses of accelerator technique and detector developments, it became possible to artificially create unstable nuclei (RI) and extract them as RI beams. Recently, research on short-lived RIs has become very active all over the world following discoveries of exotic phenomena, such as neutron halo/skin, new magic numbers and disappearance of the magic numbers. Although electron scattering should be useful even for internal structure of such Ris, it has never been applied to short-lived Ris due to difficulty for preparing target with thickness enough to perform electron scattering experiment.

To overcome this challenge, we have developed a groundbreaking technique known as SCRIT (Self-Confining Radioactive Isotope Ion Target). This innovative method leverages the ion trapping of residual gases in an electron ring, a phenomenon typically responsible for electron beam instability but ingeniously utilized in this context. Following successful commissioning, construction of the SCRIT electron scattering facility (see Fig. 1) began at the RI Beam Factory at RIKEN in 2009 and was completed in recent years.

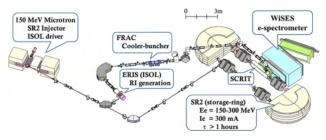


Figure 1. Overview of SCRIT electron scattering facility.

Our research has specifically focused on electron scattering experiments targeting atomic nuclei around a neutron magic number of N = 82. Notably, an experiment involving 137Cs, generated by the photofission reaction of uranium, represents the world's first electron scattering experiment with online produced RI and was published in the Physical Review Letters journal this year. Fig. 2 shows obtained momentum and angular distributions. This achievement has garnered significant attention, including a featured article in Physics Today.

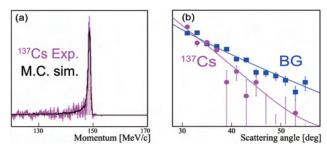


Figure 2. (a) Reconstructed momentum distribution of scattered electrons, (b) Obtained angular distribution of ¹³⁷Cs (pink) and background (blue) and theoretical calculations (solid lines).

Advanced Research Center for Beam Science – Laser Matter Interaction Science –

https://en.laser.kuicr.kyoto-u.ac.jp/



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Program-Specific Assoc Prof KANAI, Tsuneto (D Sc)



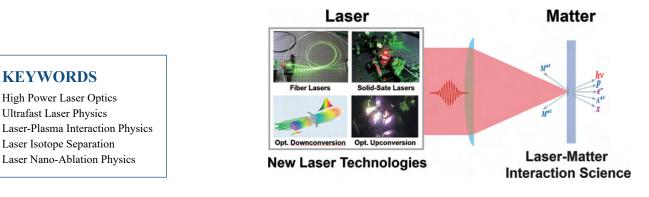
Res (pt) HASHIDA, Masaki (D Eng)

Researcher (pt)

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Scope of Research

We are developing cutting-edge high-intensity laser sources and studying experimental research on the laser interaction with matter by using the new laser sources. We are promoting cross-disciplinary research based on high-intensity laser technologies such as development of high-intensity mid-infrared solid-state lasers and fiber lasers, research on particle acceleration and wavelength conversion with plasmas produced by high-intensity ultrafast lasers, development of laser isotope separation method for neutrino research, and search for dark matter using high-intensity lasers.



Recent Selected Publications

Goya, K.; Sasanuma, H.; Ishida, G.; Uehara, H.; Tokita, S., Fusion Splicing of Plastic Optical Fibers Using a Mid-IR Fiber Laser, *Appl. Phys. Express*, **16**, 052006 (2023).

Homma, K.; Tesileanu, O.; Nakamiya, Y.; Kirita, Y.; Chiochiu, C.; Cuciuc, M.; Giubega, G.; Hasada, T.; Hashida, M.; Ishibashi, F.; Kanai, T.; Kodama, A.; Masuno, S.; Miyamaru, T.; Neagu, L.; Rodrigues, V. R. M.; Rosu, M. M.; Sakabe, S.; Tamlyn, J.; Tazlauanu, S. V.; Tokita, S., Challenge of Search for Cosmological Dark Components with High-Intensity Lasers and beyond, *Eur. Phys. J. A.*, **59**, 109 (2023).

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Li, E.; Uehara, H.; Tokita, S.; Yao, W.; Yasuhara, R., A Hybrid Quantum Cascade Laser/Fe:ZnSe Amplifier System for Power Scaling of CW Lasers at 4.0–4.6 µm, *Optics & Laser Technology*, **157**, 108783 (2023).

High-Intensity Mid-Infrared Fe:ZnSe Lasers

The mid-infrared (mid-IR) spectral region has long garnered significant interest for its spectroscopic applications. Thermal lamp-based mid-IR light sources have been traditionally employed for trace gas sensing, which is crucial for environmental monitoring, medical diagnostics, and other uses. However, the recent advancements in mid-IR broadband ultrafast lasers have paved the way for pioneering applications. These applications range from generating attosecond pulses, coherent X-ray radiation, creating high-density plasmas, and even contributing to the investigation of dark matter, in addition to their established use in molecular vibrational spectroscopy.

To achieve the desired high intensity in mid-IR lasers, optical parametric amplification (OPA) based laser systems have been the subject of extensive research in recent years. These systems necessitate the use of an ultra-high intensity nearinfrared pump laser source. They also require complex femtosecond-scale timing synchronization mechanisms. Such requirements often lead to laser systems that are inherently unstable and not user-friendly, posing significant challenges for both developers and end-users alike.

In our project, we have focused on iron-doped zinc selenide (Fe:ZnSe, as depicted in Fig. 1) as a promising laser gain medium. Fe:ZnSe exhibits a broad emission spectrum centered around the 4-micron wavelength and is capable of supporting ultrafast laser operations with a temporal duration of 100 femtoseconds. Additionally, it possesses an absorption band at the 3-micron wavelength, aligning perfectly with our home-made, world-class high-power continuous wave laser systems, such as erbium-doped ZBLAN fiber lasers and Er:YAP solid-state lasers (in collaboration with Prof. Yasuhara's group at NIFS). The Fe²⁺ ions' 3d electronic energy levels in ZnSe facilitate an upper state lifetime of approximately 100 microseconds, which obviates the need for an ultra-high intensity near-infrared pump laser source and sophisticated timing synchronization systems.

Figure 2 shows our mid-infrared laser system, which integrates a home-built seeding apparatus — comprising a Yb:CaF₂ regenerative amplifier and a three-stage KTA OPA — with an Fe:ZnSe amplifier. The entire system, which is compactly assembled on just two optical tables, would offer a robust and user-friendly platform for cutting-edge mid-IR laser research and applications.

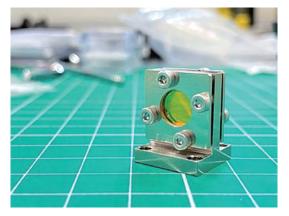


Figure 1. The picture of Fe:ZnSe laser crystal.

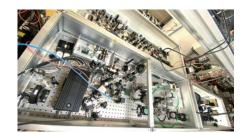


Figure 2. The picture of our mid-infrared laser system.

Blue-Violet High-Power Diode Laser System for ⁴⁸Ca Isotope Separation

In an effort to confirm the Majorana nature of neutrinos, experiments worldwide are conducting double beta decay studies without neutrino emission ($0\nu\beta\beta$ decay). Given that $0\nu\beta\beta$ decay is exceptionally rare (with an experimental lower limit half-life of approximately 10²⁶ years), it's crucial to have a substantial quantity of target nuclei in an ultra-low background setting. Among the various nuclei capable of undergoing double beta decay, ⁴⁸Ca stands out due to its highest Qvalue (4.27 MeV), surpassing natural radioactive activities, thereby promising minimal background interference. The CANDLES experiment achieved a background level of roughly 10⁻³ events/keV/yr/(kg of ^{nat}Ca), using about 305 kg of $^{nat}CaF_2$ scintillator (containing ~7.3 mol of ^{48}Ca) as the primary detector [Phys. Rev. D, 103, 092008 (2021)]. To enhance the experiment's sensitivity, isotope enrichment is imperative due to ⁴⁸Ca's low natural abundance (0.187%), along with ongoing efforts to further reduce background noise. Traditional enrichment methods like centrifugation and gas diffusion are unfeasible for ⁴⁸Ca, as it lacks a gaseous compound at room temperature, prompting the development of alternative chemical and physical techniques.

Our team is exploring a laser isotope separation (LIS) method for ⁴⁸Ca enrichment. The transition of calcium from its ground state occurs at a wavelength of approximately 422.7 nm, which can be excited using commercially available blue-violet laser diodes (LDs). The linewidth of these external cavity LDs is sufficiently narrow relative to the isotope shift in this transition, which is about several hundred MHz. However, generating around 1000 kg of ⁴⁸Ca for the experiment demands a high-power laser system exceeding kilowatts.

The gallium nitride (GaN) LD is emerging as the most promising laser source for this application due to its efficiency, compactness, longevity, reliability, and cost-effectiveness. Yet, developing a cost-effective technology that combines high power with single frequency in LDs is a challenge. For example, achieving a total optical power of 1 kW could require between 100 and 10,000 LD emitters. It's crucial that the wavelength of all emitters is precisely stabilized to match the absorption line of the ⁴⁸Ca isotope, with absolute accuracy within a few MHz to counteract the ~60 MHz Doppler broadening of the Ca atomic beam. We are currently devising a method to stabilize the wavelengths of multiple GaN-LDs simultaneously. This technique will enable the scaling of laser power by increasing the number of LDs while preserving the laser wavelength and spectral linewidth, paving the way for practical LIS applications and future isotope enrichment.

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Assist Prof (D Sc)



Program-Specific Res* NEMOTO, Takashi KIYOMURA, Tsutomu

*Nanotechnology Platform

Researcher (pt) OGAWA, Tetsuya (D Sc) **Assist Techn Staff** SUZUKI, Hiroshi

Students

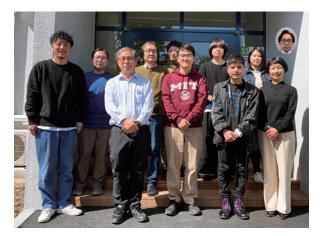
LIN, I-Ching (D3) SATO, Shinya (M2) MORIMOTO, Syunji (M2) YASUI, Kentaro (M2) JO, Yoshiyuki (M1)

Scope of Research

In the field of nanotechnology, the importance of high spatial resolution analysis of materials further increases. We study the structure and the electronic state of materials at atomic scale through direct imaging of atoms or molecules by (scanning) transmission electron microscopy ((S)TEM) combined with energy dispersive X-ray spectroscopy (EDS) and electron energy-loss spectroscopy (EELS), which gives the information of elemental and electronic state. And we are studying with the aim of establishing new analytical methods using electron microscopes and evaluating materials using these methods.

KEYWORDS STEM EELS HAADF Elemental Mapping Channeling





Recent Selected Publications

Lin, I-C.; Haruta, M.; Nemoto, T.; Goto, M.; Shimakawa, Y.; Kurata, H., Extraction of Anisotropic Thermal Vibration Factors for Oxygen from the Ti L_{2,3}-Edge in SrTiO₃, J. Phys. Chem. C., **127(36)**, 17802-17808 (2023). Supplemental cover

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Haruta, M.; Kikkawa, J.; Kimoto, K.; Kurata, H., Comparison of Detection Limits of Direct-Counting CMOS and CCD Cameras in EELS Experiments, Ultramicroscopy, 240, [113577-1]-[113577-6] (2022).

Haruta, M.; Nemoto, T.; Kurata, H., Sub-picometer Sensitivity and Effect of Anisotropic Atomic Vibrations on Ti L2,3-Edge Spectrum of SrTiO₃, Appl. Phys. Lett., 119, [232901-1]-[232901-5] (2021). Featured Article

Iwashimizu, C.; Haruta, M.; Kurata, H., Electron Orbital Mapping of SrTiO₃ Using Electron Energy-Loss Spectroscopy, Appl. Phys. Lett., 119, [232902-1]-[232902-5] (2021). Editor's Pick

Different Atomic Contrasts in HAADF Images and EELS Maps of Rutile TiO₂

High-angle annular dark-field (HAADF) imaging and elemental mapping at the atomic scale by scanning transmission electron microscopy (STEM) combined with electron energyloss spectroscopy (EELS) are widely used for material characterization. Recently, theoretical and experimental electron orbital mapping using STEM-EELS has been reported. Quantitative understanding of the contrast of the image is important to discuss the anisotropy of the orbital in an EELS map.

Figure 1 shows an experimental HAADF image with simultaneously measured Ti-L2.3 and O-K elemental maps and the simulated elemental maps. Only the Ti atomic columns are visualized in the HAADF image due to its Z-contrast nature. The Ti and O elemental map measured using EELS show the respective atomic columns (Fig. 1c and d). The O map shows the distorted projected octahedral structure that agrees with the structure model (Fig. 1a), and the atomic shape is an isotropic distribution. On the other hand, the shape of the atom in the Ti map shows an anisotropic elliptical distribution that extends along the long axis of the octahedron, even though the HAADF image does not show such anisotropic contrast. Figures 1e and 1f show the simulated images of O and Ti elemental maps for the same sample thickness as experiment (32 nm). The Ti $L_{2,3}$ -map shows anisotropic atomic shape along the long axis of the octahedron like the experimental one. This indicates that Ti maps of TiO₂ can show an anisotropic elliptical shape, regardless of the anisotropic electron orbital, because the simulation program (µSTEM) assumes (isotropic) isolated atoms without bonding character. We investigated the electron channeling process to elucidate the cause of the difference of the Ti atomic shape between the HAADF image and Ti L_{23} -map. Figure 2 shows the probe intensity propagating along the [001] axis of a rutile TiO₂ crystal as a function of the thickness, where the cross-section image is observed from the [110] direction along the black line indicated in Fig. 1. Figure 2a-e corresponds to the probe positions as numbered on the top. When the probe is located on a Ti (Fig. 2a and e) or O (Fig. 2c) column, strong electron channeling occurs, by which the incident electrons travel straight along each column. In the case of position 2 (Fig. 2b), the probe incident near an O column is quickly channeled onto the nearby oxygen atomic column. This can be confirmed by the high intensity in the O elemental map (Fig. 1c and 1e) and the low intensity in the Ti elemental map (Fig. 1d and 1f) at the yellow position, which corresponds to probe position 2. On the other hand, in the case of position 4 (Fig. 2d), the probe incident near a Ti column is also channeled onto a nearby Ti column. Therefore, the Ti $L_{2,3}$ edge is highly excited at position 4 due to the delocalization of inelastic scattering (Fig. 2d), whereas the excitation is suppressed at position 2 due to channeling onto the nearby oxygen column (Fig. 2b). It is considered that these processes are main reason for the anisotropic contrast in Ti $L_{2,3}$ -map.

It is shown that considering the anisotropic shape of Ti atomic column observed in the Ti elemental map is essential for the quantification and visualization of electron orbitals. Consequently, much care must be taken in interpreting EELS maps.

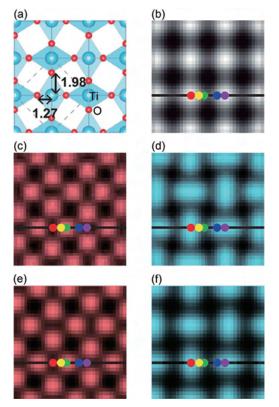


Figure 1. (a) Projected structure model of rutile TiO_2 along the [001] axis. The dashed line shows the unit cell. The lengths of the long and short Ti–O bond in the projected TiO₆ octahedron is written. (b) Accumulated experimental HAADF image. Elemental maps of (c) O *K*- and (d) Ti $L_{2,3}$ -edges. Simulated elemental maps of (e) O *K*- and (f) Ti $L_{2,3}$ -edges. The black lines in (b–f) and colour points correspond to the probe positions in Fig. 2.

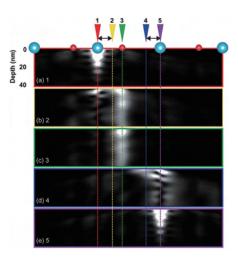


Figure 2. Probe intensity as a function of thickness in the [001]-oriented rutile TiO_2 crystal, where the cross-section image was observed from the [110] direction along the black lines indicated in Fig. 1. The electron probes are located on each triangle labelled 1–5, which correspond to the coloured dots in Fig. 1. (a, e) Probe located on the Ti column and (c) on the O column. The distances between positions 1 and 2 and between positions 4 and 5 are the same. This distance corresponds to the half width at half maxima of the short axis of the elliptical shape of the Ti map. Ti and O atoms are indicated as blue and red circles, respectively.

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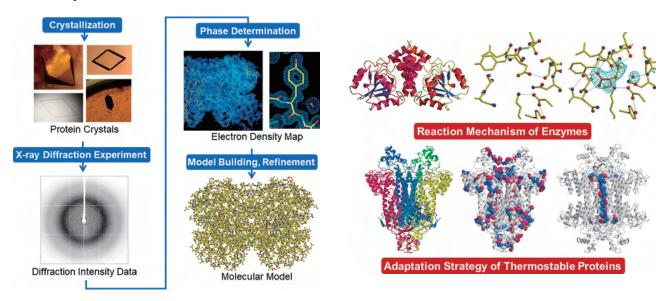
Assist Prof FUJII, Tomomi (D Sc)

Scope of Research

This laboratory analyzes X-ray crystallographic structures of biological macromolecules and studies the structural biology about the relationships between protein structures and their functions and properties based on the crystal structures. The main research themes are elucidation of the reaction mechanism of enzymes, the relationship between the multiform conformation and the functional variety of proteins, the structural basis for the domain-arrangements of multi-domain proteins or proteinprotein interactions, structure determination for structure-based protein engineering and industrial application, and the adaptation strategy of proteins from thermophilic or cold-adapted bacteria.

KEYWORDS

Crystal X-ray Crystallographic Analysis Structural Biology Protein Crystallography Structure and Function



Recent Selected Publications

Fujii, T.; Sato, A.; Okamoto, Y.; Yamauchi, T.; Kato, S.; Yoshida, M.; Oikawa, T.; Hata, Y., The Crystal Structure of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005 Provides Insights into the Reaction Mechanism of Enzymes in Its Original Family, *Proteins: Structure, Function, and Bioinformatics*, **84**, 1029-1042 (2016).

Fujii, T.; Yamauchi, T.; Ishiyama, M.; Gogami, Y.; Oikawa, T.; Hata, Y., Crystallographic Studies of Aspartate Racemase from *Lactobacillus* sakei NBRC 15893, Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun., **71**, 1012-1016 (2015).

Fujii, T.; Goda, Y.; Yoshida, M.; Oikawa, T.; Hata, Y., Crystallization and preliminary X-ray Diffraction Studies of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **64**, 737-739 (2008).

Fujii, T.; Oikawa, T.; Muraoka, I.; Soda, K.; Hata, Y., Crystallization and Preliminary X-ray Diffraction Studies of Tetrameric Malate Dehydrogenase from the Novel Antarctic Psychrophile *Flavobacterium frigidimaris* KUC-1, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **63**, 983-986 (2007).

Fujii, T.; Sakai, H.; Kawata, Y.; Hata, Y., Crystal Structure of Thermostable Aspartase from *Bacillus* sp. YM55-1: Structure-based Exploration of Functional Sites in the Aspartase Family, *J. Mol. Biol.*, **328**, 635-654 (2003).

Refined Crystal Structure of the Oxygenase Component (GraA) of Resorcinol Hydroxylase

Resorcinol hydroxylase is involved in the first step of the resorcinol catabolic pathway and catalyzes the hydroxylation of resorcinol to hydroxyquinol. This enzyme belongs to the two-component flavin-diffusible monooxygenase (TC-FDM) family and comprises two components: an oxygenase and a flavin reductase. It uses molecular oxygen and reduced flavin for hydroxylation and NAD(P)H for flavin reduction. The smaller component, flavin reductase, generates reduced flavin to allow the oxygenase component to oxygenate the substrate. Thus, the enzymatic reaction is executed in two steps. However, hydroxylation activity requires cooperation between both the components. To understand the structural basis of the catalytic mechanism, we performed a crystal structure analysis of the apo-form of the oxygenase component (GraA) from Rhizobium sp. strain MTP-10005. GraA is a tetramer, and its subunit consists of 409 amino acid residues with a mass of 43,305 Da.

N-terminal His-tagged GraA was used for crystallization. The protein solution consisted of 5 mg/ml GraA and 50 mM Tris-HCl pH 8.0. Crystals with suitable sizes for X-ray diffraction experiments were obtained over several days by a sitting drop vapor diffusion method, with a reservoir solution consisting of 17% (w/v) PEG3350 and 0.2 M K₂HPO₄. They belonged to the tetragonal space group $I4_{1}22$ with unit cell dimensions of a = b = 101.6 Å, c = 319.8 Å and contained one GraA subunit in asymmetric unit. Diffraction data were collected up to 1.9 Å resolution under cryogenic conditions at beamline BL5A, PF, Tsukuba, Japan. The structure was determined by molecular replacement and refined at 1.9 Å resolution up to R = 0.162 and $R_{free} = 0.185$.

GraA is a tetramer of four identical subunits related to one another by three molecular two-fold axes which are identical to crystallographic two-fold axes (Figure 1). A given pair of two subunits in the molecule forms a close dimer and two of the close dimers form a loose dimer. The GraA tetrameric molecule adopts the structure of a dimer of dimers. The subunit consists of three domains (Figure 2). The N-terminal domain (residues Met1-Ala121) has an α -structure mainly of antiparallel α -helices, the central domain has a β -structure of two β -sheets stacked together, and the C-terminal domain (residues Phe218-Tyr409) has a four-helix-bundle structure of long antiparallel α -helices involved in tetramer formation. The part of PEG3350 used as a precipitating agent for the crystallization is located in the space that is encompassed by these three domains (Figure 2). The PEG binds to both the binding site of a portion of isoalloxazine ring of FAD in the GraA-FAD complex and the putative substrate binding site (Figure 3). The loop region of 13 residues (residues Gly271–Asn283), which is ordered and covers the FAD of another subunit in the GraA-FAD complex, is disordered in this apo-form (Figures 2 and 3).

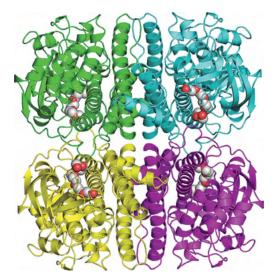


Figure 1. Tetrameric molecular structure of the apo-form of the oxygenase component of resorcinol hydroxylase (GraA) from *Rhizobium* sp. strain MTP-10005 with bound PEG.

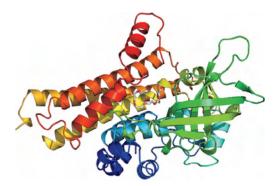


Figure 2. Subunit structure of the apo-form of the oxygenase component of resorcinol hydroxylase (GraA) from *Rhizobium* sp. strain MTP-10005 with bound PEG.

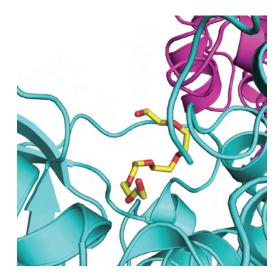


Figure 3. Structure of the active site cleft of the apo-form of the oxygenase component of resorcinol hydroxylase (GraA) from *Rhizobium* sp. strain MTP-10005 with bound PEG.

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Program-Specific Assist Prof MINEO, Keito (D Agr)

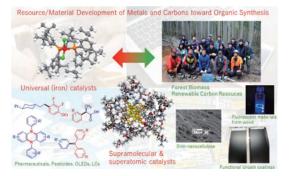
Researchers (pt)

IMAI, Makiko MATSUMURA, Hiroyuki AOKI, Satoshi

Scope of Research

AVENA, Ramon Francisco Bernardino NAKAMURA, Yuki

Our research activity focuses on the development of new molecular transformations, which can contribute to better or ideal synthesis of functional molecules as well as to exploitation of new chemical (metal and carbon) resources. The present research subjects are (1) metal-catalyzed carbon–carbon and carbon–heteroatom bond forming reactions by using universal metals such as iron (2) development of small metallic nanocluster catalysts based on supramolecular approaches (3) utilization of woody biomass as the renewable carbon resources by mild catalytic transformations of wood molecules into useful compounds and materials.



KEYWORDS

Iron Catalysis Orga

Organotransformation Woody Molecular Transformation

formation Supramolecular & Superatomic Catalysis

Recent Selected Publications

Isozaki, K.; Iseri, K.; Saito, R.; Ueda, K.; Nakamura, M., Dual Catalysis of Gold Nanoclusters: Photocatalytic Cross-Dehydrogenative Coupling by Cooperation of Superatomic Core and Molecularly Modified Staples, *Angew. Chem. Int. Ed.* (in press).

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Isozaki, K.; Ueno, R.; Ishibashi, K.; Nakano, G.; Yin, H.; Iseri, K.; Sakamoto, M.; Takaya, H.; Teranishi, T.; Nakamura, M., Gold Nanocluster Functionalized with Peptide Dendron Thiolates: Acceleration of the Photocatalytic Oxidation of an Amino Alcohol in a Supramolecular Reaction Field, *ACS Catal.*, **11**, 13180-13187 (2021).

Adak, L.; Jin, M.; Saito, S.; Kawabata, T.; Itoh, T.; Ito, S.; Sharma, A. K.; Gower, N. J.; Cogswell, P.; Geldsetzer, J.; Takaya, H.; Isozaki, K.; Nakamura, M., Iron-Catalysed Enantioselective Carbometalation of Azabicycloalkenes, *Chem. Commun.*, **57**, 6975-6978 (2021).

Agata, R.; Takaya, H.; Matsuda, H.; Nakatani, N.; Takeuchi, K.; Iwamoto, T.; Hatakeyama, T.; Nakamura, M., Iron-Catalyzed Cross Coupling of Aryl Chlorides with Alkyl Grignard Reagents: Synthetic Scope and FeII/FeIV Mechanism Supported by X-Ray Absorption Spectroscopy and Density Functional Theory Calculations, *Bull. Chem. Soc. Jpn.*, **92**, 381-390 (2019).

Iron-Catalyzed Organic Synthesis

Development of organic transformations using earth abundant transition-metals is becoming more and more important in recent years. Our group focuses on use of iron as a catalyst, and so far developed a variety of iron-catalyzed cross-coupling reactions, some of which can't be achieved by conventional transition-metal catalysts such as palladium. As a recent representative example, we developed a new bisphosphine ligand, SciPROP-R which enables facile iron-catalyzed Suzuki-type cross-coupling between alkyl chlorides and arylboronates. Based on the mechanistic studies, we proposed a catalytic cycle in which SciPROP-R ligand facilitates the smooth halogen abstraction from alkyl chlorides. Also, we have developed a magnetite nanoparticle-catalyzed oxidation reaction of primary and secondary alcohols assisted by microwave irradiation (Figure 1). Magnetite nanoparticles have the additional advantage of being easily recoverable from the reaction mixture by magneto-separation, which allows them to be successively recycled several times with negligible loss in activity.

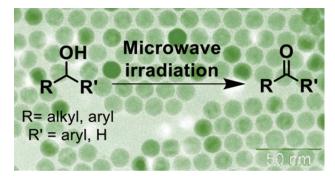


Figure 1. Microwave-assisted oxidation of alcohols catalyzed by ironoxide nanoparticles.

Supramolecular & Superatomic Catalysis

This project focuses on the development of highly active and selective metallic nanoparticle and cluster catalysts. To achieve this purpose, four key methodologies have been developed: 1) creation of reaction field with advanced self-assembly, 2) design of selective molecular transformation with multi-points intermolecular interaction, 3) size selective synthesis of metallic nanoparticles and clusters, and 4) utilization of plasmonic resonance with light. As a recent representative example, we reported a new finding of dual catalytic property of gold nanoclusters originating from two structural components, superatomic core and surrounding staples. The cooperative catalysis enables the cross coupling between photooxidized iminium intermediates and alkynyl-gold species, providing propargylamine derivatives.

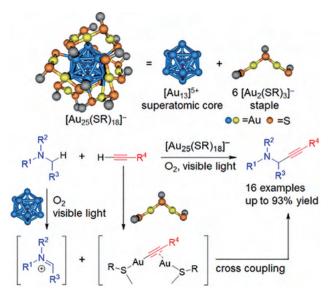


Figure 2. Dual catalysis of gold nanoclusters toward photocatalytic cross-dehydrogenative coupling between tertiary amines and terminal alkynes.

Wood Molecular Transformation

Woody biomass is renewable and the most abundant carbon resource on the earth, thus expected to utilize as a feedstock to chemicals and energy toward a sustainable society. This project focuses on the chemical transformation of woody biomass into useful materials under mild catalytic conditions. To achieve this purpose, we have developed two key technologies; 1) direct transformation of woody lignin to fluorescent molecules, 2) one-pot disintegration of wood powder into nanocellulose. As a recent representative example, we reported the development of artificial urushi-coating materials by installing trienyl side chains from natural linolenic acid to the bio-renewable phenoxypropanone compounds obtained from enzymatic degradation of woody lignin.

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Prof SHIMAKAWA, Yuichi (D Sc)



Assoc Prof KAN, Daisuke (D Sc)



Assist Prof GOTO, Masato (D Sc)



Techn Staff ICHIKAWA, Noriya (D Eng)

Students

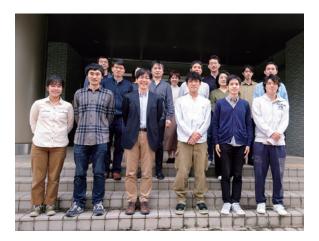
IIHOSHI, Makoto (D2) ISODA, Yosuke (D2) SHEN, Yufan (D2) XIE, Lingling (D2) CHEN, Chen (D2) WATANABE, Rei (D1) ITO, Mayuri (M1) FUJI, Souta (M1)

Scope of Research

Transition metal oxides have a wide variety of interesting and useful functional properties, including electronic conduction, superconductivity, ferroelectricity, and ferromagnetism. In fact, some of these oxides are used in current electronic devices. Our research mainly focuses on perovskite-structured transition metal oxides with novel functional properties due to complex couplings between their lattices, charges and spins. We are currently exploring such functional oxides with advanced oxide-synthesis techniques such as high-pressure synthesis and epitaxial thin film growth.

KEYWORDS

Solid State Chemistry High Pressure Synthesis Heterointerface Functional Metal Oxides Epitaxial Thin Film Growth



Recent Selected Publications

Iihoshi, M.; Goto, M.; Kosugi, Y.; Shimakawa Y., Cascade Charge Transitions of Unusually High and Mixed Valence Fe^{3.5+} in the A-Site Layer-Ordered Double Perovskite SmBaFe₂O₆, *J. Amer. Chem. Soc.*, **145**, 10756-10762 (2023).

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Isoda, Y.; Kan, D.; Majima, T.; Shimakawa Y., Orientation-Dependent Electrochemical Reduction and Proton Evolution in the Oxygen-Deficient Perovskite SrFeO_{2.5+y}, *Appl. Phys. Express*, **16**, 015506/1-5 (2023).

Cascade Charge Transitions of Unusually High and Mixed Valence Fe^{3.5+} in the A-Site Layer-Ordered Double Perovskite SmBaFe₂O₆

Phase transitions caused by relieving of charge instability are one of the most important and interesting phenomena in solid state chemistry and condensed matter physics. A typical example was found in Fe₃O₄, and the transition is often called the Verwey transition. It occurs when the instability of a mixed valence state of Fe^{2.5+} at the B site of the spinel-type crystal structure is relieved, resulting in charge-ordered states of Fe²⁺ and Fe³⁺, with an accompanying metal-to-insulator transition. Another phase transition caused by relieving charge instability is seen in compounds containing an unusually high valence state of ions. The typical example is Fe⁴⁺ seen in the perovskite-type structured CaFeO₃. Fe⁴⁺ in CaFeO₃ shows charge disproportionation to Fe3+ and Fe5+ in a rock-salt manner, which accompanies a metal-to-insulator transition. We are then very interested in the phase transition behaviors of a compound containing ions in both unusually high and mixed valence states. To prepare such a compound, in this work, we used the A-site layer-ordered oxygen-deficient precursor SmBaFe₂O₅, which contains the mixed valence state of Fe^{2.5+} ions. By topochemically oxidizing the compound to fully incorporate oxygen ions into the vacant sites, the A-site layer-ordered double perovskite SmBaFe₂O₆ with the unusually high and mixed valence state of Fe^{3.5+} was obtained. We have found that cascade phase transitions are induced in SmBaFe₂O₆ to relieve the charge instability, described as SmBaFe^{3.5+}₂O₆ \rightarrow SmBa(Fe³⁺Fe⁴⁺)O₆ \rightarrow $SmBa(Fe^{3+}Fe^{(4-\delta)+}_{0.5}Fe^{(4+\delta)+}_{0.5})O_{6} \rightarrow SmBa(Fe^{3+}_{1.5}Fe^{5+}_{0.5})O_{6}.$ The first Verwey-like charge-order transition occurred at 340 K and was accompanied by a significant structural change and a sudden increase in magnetic susceptibility. The following transition was the charge disproportionation of metastable Fe⁴⁺ to Fe³⁺ and Fe⁵⁺, and each of the spins resulted in the antiferromagnetic ground state.

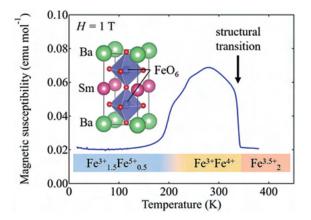
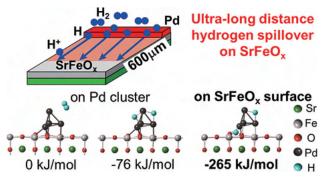
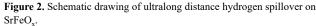


Figure 1. Crystal structure of the topochemically oxidized double perovskite $SmBaFe_2O_6$ and temperature dependence of magnetic susceptibility of $SmBaFe_2O_6$.

Ultralong Distance Hydrogen Spillover Enabled by Valence Changes in a Metal Oxide Surface

The surface of metal oxides is a fertile platform for chemical reactions and an important subject of investigation. However, experimentally characterizing and understanding surface reactions are challenging, especially when hydrogen is involved in chemical reactions on oxides' surfaces. The occurrence of hydrogen spillover on oxide surfaces has been established since its discovery in 1964. Furthermore, this phenomenon has been utilized as a reaction route for producing functional materials. Nonetheless, the fundamental characteristics of hydrogen spillover remain elusive. This is because of experimental difficulties in observing hydrogen during chemical reactions. In addition, reaction systems utilizing hydrogen spillover are complex and not well defined. Delineating hydrogen reactions and diffusion on oxide surfaces therefore requires proper design and construction of model (or ideal) reaction systems without such complexities. Recent progress in nanometer-level material techniques enables the fabrication of well-defined model catalytic systems with separated functions. The model systems, consisting of epitaxial films of catalytic oxide supports and metal catalysts located at controlled positions on the supports' surfaces, are useful for evaluating various phenomena associated with (electro) chemical reactions. Since catalytic supports are reduced in the hydrogen spillover process, tracking hydrogen-spilloverinduced changes in model systems enables the "visualization" of hydrogen. Here, in this study, we fabricated catalytic model systems based on Pd-loaded SrFeO_x (x~2.8) epitaxial films and investigated hydrogen spillover. We show that hydrogen spillover on the SrFeO_x support extends over long distances (~600 µm). Furthermore, the hydrogenspillover-induced reduction of Fe⁴⁺ in the support yields large energies (as large as 200 kJ/mol), leading to the spontaneous hydrogen transfer and driving the surprisingly ultralong hydrogen diffusion. These results show that the valence changes in the supports' surfaces are the primary factor determining the hydrogen spillover distance.





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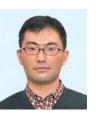
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Scope of Research

Developing efficient energy storage systems and innovative material production processes is a significant challenge for chemists to contribute to a sustainable society. We plan to approach these problems by using *transition metal clusters* of which multiple metal atoms work together as catalysts and functional materials. Our laboratory focuses explicitly on creating a new method to synthesize the clusters with atomic precision and applying the obtained clusters to difficult reactions such as the reduction of CO_2 and N_2 .

KEYWORDS

Transition Metal Clusters Homogeneous Catalysis Nitrogen Fixation Bioinorganic Chemistry



Recent Selected Publications

Izu, H.; Bhave, D. G.; Matsuoka, Y.; Sameera, W. M. C.; Tanifuji, K.; Ohki, Y., Synthesis, Characterization, and Catalytic Activity of a Cubic [Mo₃S₄Pd] Cluster Bearing Bulky Cyclopentadienyl Ligands, *Eur. J. Inorg. Chem.*, **26**, e202300399 (2023).

Ohki, Y.; Munakata, K.; Matsuoka, Y.; Hara, R.; Kachi, M.; Uchida, K.; Tada, M.; Cramer, R. E.; Sameera, W. M. C.; Takayama, T.; Sakai, Y.; Kuriyama, S.; Nishibayashi, Y.; Tanifuji, K., Nitrogen Reduction by the Fe Sites of Synthetic [Mo₃S₄Fe] Cubes, *Nature*, **607**, 86-90 (2022). Lee, C. C.; Kang, W.; Jasniewski, A. J.; Stiebritz, M. T.; Tanifuji, K.; Ribbe, M. W.; Hu, Y., Evidence of Substrate Binding and Product Release

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Tanifuji, K.; Sakai, Y.; Matsuoka, Y.; Tada, M.; Sameera, W. M. C.; Ohki, Y., CO Binding onto Heterometals of [Mo₃S₄M] (M = Fe, Co, Ni) Cubes, *Bull. Chem. Soc. Jpn.*, **95**, 1190-1195 (2022).

Tanifuji, K.; Ohki, Y., Metal-Sulfur Compounds in N2 Reduction and Nitrogenase-Related Chemistry, Chem. Rev., 120, 5194-5251 (2020).

Catalytic N₂ Silylation by the Fe Sites of Cuboidal [Mo₃S₄Fe] Clusters

Biological N₂ fixation is conducted by nitrogenase that employs a unique Fe/Mo-S-C cluster as its catalytic site (FeMoco, [(R-homocitrate)MoFe₇S₉C]). Synthetic counterparts of the FeMoco, metal-sulfur clusters, demonstrated capturing N₂ on rare occasions; nevertheless, the catalytic conversion of this stable molecule has not been achieved despite its relevance to the biological N₂ fixation. This study focuses on capture, activation, and catalytic conversion of N_2 by an Fe atom incorporated into our $[Mo_3S_4]$ incomplete-cubane platform bearing bulky Cp ligands. Treatment of these clusters with excess Na and ClSiMe₃ under a N₂ atmosphere gave N(SiMe₃)₃ with up to 248 eq. per cluster. This work exemplifies the N2-reducing capability of Fe atoms in a S-rich environment, which biological systems have selected to achieve a similar purpose. Further studies are ongoing to unveil the effect of an incorporated metal atom (Fe vs Co or Ni) on catalytic N2 silvlation.

Figure 1. Proposed N_2 binding state of FeMoco and a $\mathrm{N}_2\text{-bound}$ Mo-Fe-S cluster.

Tracing the S Incorporation into the Nitrogenase Cofactor Precursor

FeMoco is arguably one of the most complex metallocofactors in Nature. Its biosynthetic pathway is correspondingly complicated and remains unclear, which hampers applications of this enzyme toward artificial N₂ fixation. In this study, we investigated an enzymatic process by which FeMoco precursor (L-cluster, [Fe₈S₉C]) is generated from two [Fe₄S₄] clusters on the protein by using a *semi-synthetic* approach. The study revealed that this process includes a S atom uptake from SO₃²⁻ and that the S atom is replaceable with homologous elements (Se, Te). Moreover, we succeeded in selective observation of the incorporated elements and theoretical simulations supporting the reactions' feasibility. These results show that nitrogenase requires an S source as an external substrate for its function.

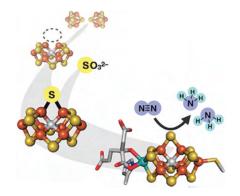


Figure 2. Schematic description of a sulfur uptake from sulfite (SO_3^{2-}) in the biosynthetic pathway of FeMoco.

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Scope of Research

Our research interest is to understand optical and quantum properties of nanometer-structured materials and to establish opto-nanoscience for creation of innovative functional materials. Space- and time-resolved laser spectroscopy is used to study optical properties of semiconductor quantum nanostructures and strongly correlated electron systems in lowdimensional materials. The main subjects are as follows: 1) investigation of optical properties of single nanostructures through the development of a high-resolution optical microscope, 2) ultrafast optical spectroscopy of excited states of semiconductor nanostructures, 3) photophysics of solar cell materials, and 4) engineering material properties with lights.

KEYWORDS

Femtosecond Laser Spectroscopy Quantum Dots High Harmonic Generation

Single Photon Spectroscopy Perovskites



Recent Selected Publications

Zhang, Z.; Sekiguchi, F.; Moriyama, T.; Furuya, S. C.; Sato, M.; Satoh, T.; Mukai, Y.; Tanaka, K.; Yamamoto, T.; Kageyama, H.; Kanemitsu, Y.; Hirori, H., Generation of Third-Harmonic Spin Oscillation from Strong Spin Precession Induced by Terahertz Magnetic Near Fields, Nature Commun., 14, [1795-1]-[1795-7] (2023).

Nakagawa, K.; Hirori, H.; Sato, S. A.; Tahara, H.; Sekiguchi, F.; Yumoto, G.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Size-Controlled Quantum Dots Reveal the Impact of Intraband Transitions on High-Order Harmonic Generation in Solids, Nature Phys., 18, 874-878 (2022).

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Yumoto, G.; Hirori, H.; Sekiguchi, F.; Sato, R.; Saruyama, M.; Teranishi, T.; Kanemitsu, Y., Strong Spin-Orbit Coupling Inducing Autler-Townes Effect in Lead Halide Perovskite Nanocrystals, Nature Commun., 12, [3026-1]-[3026-7] (2021).

Sekiguchi, F.; Hirori, H.; Yumoto, G.; Shimazaki, A.; Nakamura, T.; Wakamiya, A.; Kanemitsu Y., Enhancing the Hot-Phonon Bottleneck Effect in a Metal Halide Perovskite by Terahertz Phonon Excitation, Phys. Rev. Lett., 126, [077401-1]-[077401-6] (2021).

The Second- and Third-Harmonic Generation from Spin Precession in a Canted Antiferromagnet

Recently, antiferromagnetic spintronics is considered as one of the important next-generation information technologies, owing to the low-loss and non-volatility of spin properties. Therefore, the spin dynamics in antiferromagnets with the resonance at terahertz (THz) frequencies, has attracted much interest. However, because of the lack of strong THz magnetic fields, the THz spin dynamics has not yet been well understood. In this study, we developed a novel micro-resonator to efficiently enhance the magnetic component of THz wave, which allows the generation of the world's strongest THz magnetic field up to 2 Tesla in an antiferromagnet HoFeO3.1) By using this strong THz magnetic field, we succeeded in inducing the unprecedentedly large magnetization change and thus generating the second and third harmonics of fundamental spin frequency (Fig. 1), for the first time. Furthermore, our research provides a deep understanding of relationship between the harmonics and the spin structure. The efficient excitation method of spin dynamics and the understanding of nonlinear spin dynamics can help us establish novel nonlinear spintronics at terahertz frequencies.

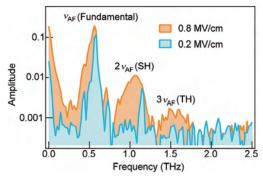


Figure 1. Spectrum of spin dynamics. Different colors indicate different excitation powers.

Size-Dependent Structural Phase Transition in Single Lead Halide Perovskite Nanocrystals

Lead halide perovskite nanocrystals (NCs) have attracted attention as a new light-emitting material because of their high photoluminescence (PL) quantum yields and bandgap tunability around the whole visible region. Halide perovskites have three crystal structures (orthorhombic, tetragonal, and cubic), and the PL peak energy depends strongly on the crystal structure. However, it is unclear how the NC size affects the phase transition temperature. In this study, we investigated the temperature dependence of the PL spectra in single perovskite APbBr₃ (A = FA (HC(NH₂)₂) and Cs) NCs from 5.5 to 200 K using single-dot PL spectroscopy.²⁾ For FAPbBr₃ NCs, a redshift in PL peak energy due to the orthorhombic to tetragonal phase transition is observed between 100 and 150 K, while CsPbBr₃ NCs show no phase transition within the observed temperature range. We found that the phase transition temperature decreases in smaller FAPbBr₃ NCs (Fig. 2).

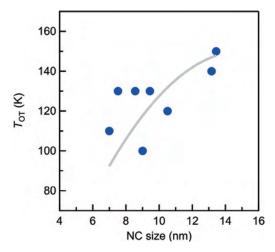


Figure 2. Size dependent orthorhombic-to-tetragonal phase transition temperature (T_{OT}) in FAPbBr₃ NCs.

Anomalous Band-Edge Optical Responses in a Two-Dimensional Ferroelectric Halide Perovskite

In two-dimensional (2D) halide perovskites, electrons and holes confined in atomically thin 2D perovskite layers form excitons with extremely large binding energies. The peculiar optical properties emerge from such stable excitons. In addition, because the lattice distortion of the perovskite structure can be controlled by the organic molecular cations contained in 2D halide perovskites, the unique structural properties appear: Large lattice distortion introduced by large-sized organic cations results in the emergence of ferroelectricity in 2D halide perovskites. Therefore, clarifying the correlation between the crystal structure and optical properties is important for understanding the physical properties of ferroelectric halide perovskites and developing new devices. In this study, we measured the temperature dependences of the absorption spectra, second harmonic generation (SHG) intensity, and lattice constants of 2D ferroelectric perovskite (BA)₂(EA)₂Pb₃I₁₀ single crystals (BA is n-butylammonium and EA is ethylammonium).³⁾ We found the anomalous temperature behavior of the Urbach tail of the absorption spectrum exhibiting a significant change at around 200 K. We revealed that this change is correlated with the temperature dependences of the SHG intensity and the in-plane lattice distortion. We concluded that the randomness of the ferroelectric polarizations modifies the linewidth of the band-edge exciton transition and leads to the anomalous temperature dependence of the steepness parameter of the Urbach tail.

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2) K. Cho, T. Yamada, M. Saruyama, R. Sato, T. Teranishi, and Y. Kanemitsu, *J. Chem. Phys.* **158**, 201104 (2023).

3) C. Higashimura, G. Yumoto, T. Yamada, T. Nakamura, F. Harata, H. Hirori, A. Wakamiya, and Y. Kanemitsu, *J. Phys. Chem. Lett.* **14**, 8360 (2023).

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Scope of Research

We are interested in understanding the functioning and evolution of biological systems at varying scales from tiny microbes up to the Earth's environment, by leveraging rapidly accumulating big data in life science and bioinformatics approaches. We currently focus on 1) the evolution of viruses and their links to the origin of life, 2) microbial ecology in different ecosystems, and 3) the development of bioinformatics methods and biological knowledge resources for biomedical and industrial applications. To fuel these research activities, we take part in environmental sampling campaigns such as Tara Oceans. Our resources and developed tools are accessible through GenomeNet (www.genome.jp) to scientific communities and the public.



KEYWORDS GenomeNet **Bioinformatics Environmental Genomics**

Virology

Molecular Evolution

Recent Selected Publications

Gaïa M.; Meng L.; Pelletier E.; Forterre P.; Vanni C.; Fernandez-Guerra A.; Jaillon O.; Wincker P.; Ogata H.; Krupovic M.; Delmont, T. O., Mirusviruses Link Herpesviruses to Giant Viruses, Nature, 616, 783-789 (2023).

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Kaneko H.; Endo H.; Henry H.; Berney C.; Mahé F.; Poulain J.; Labadie K.; Beluche O.; El Hourany R.; Tara Oceans Coordinators, Chaffron S.; Wincker P.; Nakamura R.; Karp-Boss L.; Boss E.; Bowler C.; de Vargas C.; Tomii K.; Ogata H., Predicting Global Distributions of Eukaryotic Plankton Communities from Satellite Data, ISME Commun., 3, 101 (2023).

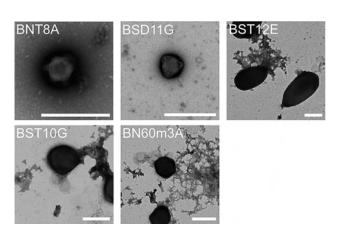
Meng L.; Delmont T. O.; Gaïa M.; Pelletier E.; Fernandez-Guerra A.; Chaffron S.; Neches R. Y.; Wu J.; Kaneko H.; Endo H.; Ogata H., Genomic Adaptation of Giant Viruses in Polar Oceans, Nat. Commun., 14, 6233 (2023).

Isolation and Whole Genome Sequencing of Giant Viruses from Lake Biwa, Japan

Giant viruses are double-stranded DNA viruses with extremely large genomes and particles reaching 2.5 megabases and 1.5 µm, respectively. These viruses are ubiquitous in the environment and important drivers for nutrient cycles. Currently, various giant viruses have been isolated, but whole-genome sequences of these viruses are limited because of sequencing costs. Here, we evaluated accuracy of giant virus genome assembly by MinION sequencing, which enables rapid and low-cost sequencing. As MinION sequencing produces error-prone reads, the assembly process generally requires correction by other sequencing platforms. However, recent studies assembled high-quality microbial genomes by MinION sequencing alone. We confirmed that genome assembly constructed by MinION sequencing alone is highly accurate for giant viruses with over 99.98% identity to the reference genome by re-sequencing a prototype giant virus. As a proof of concept, we further sequenced five giant viruses isolated from Lake biwa, Japan, by using MinION sequencing. Comparison between newly assembled genomes and reference genomes revealed that these isolates represent new species of marseillevirus, pithovirus, and mimivirus. Overall, we propose that genome assembly by MinION sequencing alone is an effective approach for a genome-wide analysis of isolated giant viruses. This research was published in a journal, Environmental microbiology (doi: 10.1111/1462-2920.16476).

A Giant Endogenous Viral Element: Evidence of Recent Infection of a Double-Stranded DNA Virus in a Fungus

Fungal virosphere is dominated by RNA viruses, with few single-stranded DNA viruses. So far, no double-stranded DNA virus has been identified in fungi. Rhizophagus irregularis is a species of arbuscular mycorrhizal fungus, belonging to the class Glomeromycetes. We searched viral signals within chromosome-level genomic assemblies of five different strains of this fungi species. On chromosome 8 of a strain 4401, we discovered a 1.5-megabase region, which showed distinct features from other chromosomal regions with strong viral signals. This viral region harbors five Nucleocytoviricota marker genes. Our phylogenetic analysis revealed that these genes are closely related to Asfarviridae sequences (Fig. 1). These marker genes remain in single copy and show the same tree topology, which suggest that this viral region originated from a single viral integration event. In the chromosomes of other strains, this viral region is absent. Also, the content of repetitive sequences and transposable elements in this viral region is lower compared to other genomic regions. These findings suggest that the viral region was inserted after the divergence of five R. irregularis strains. This work has been published in Zhao et al., Virus Evolution, 2023, doi: 10.1093/ ve/vead064.



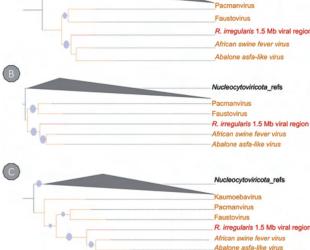


Figure 1. Isolated giant viruses observed under transmission electron microscopy. Names of isolates were shown top left. BNT8A and BSD11G are marseilleviruses. BST12E is a pithovirus. BST10G and BN60m3A are mimiviruses. Bars indicate 500 nm. This figure is modified from that published in Hikida et al. (2023) *Environ. Microbiol.* under the CC BY 4.0 license.

Figure 2. Phylogenetic trees based on core genes of viruses of the phylum *Nucleocytoviricota* based on maximum-likelihood frameworks. Blue circles represent supports that passed confidence cutoff for branches. Yellow represents asfarviruses, and red indicates sequences from the viral region. (a) Concatenated tree of three polymerases. (b) Tree of mRNA capping enzyme (c) Tree of viral late transcription factor 3.

Nucleocytoviricota refs

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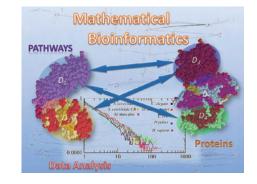
ZHAO, Jiaying	The University of Hong Kong, Hong Kong, 31 May 2023–21 August 2023
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HAN, Mingjing	Nankai University, China, 22 August 2023–31 May 2024
ZHONG, Yezhao	National University of Ireland, Galway, Ireland, 6 November 2023-26 January 2024
HSU, Zi-Chu	National Yan Ming Chiao Tung University, Taiwan, 25 November 2023–15 December 2023
CHEN, Tze-Shin	National Yan Ming Chiao Tung University, Taiwan, 25 November 2023–15 December 2023
TUNG, Cheng-Yu	National Yan Ming Chiao Tung University, Taiwan, 25 November 2023–15 December 2023

Scope of Research

Due to the rapid progress of genome sequencing technology, whole genome sequences of organisms ranging from bacteria to human have become available. In order to understand the meaning behind the genetic code, we have been developing algorithms and software tools for analyzing biological data based on advanced information technologies such as theory of algorithms, artificial intelligence, and machine learning. We are currently studying the following topics: systems biology, scale-free networks, protein structure prediction, the inference of biological networks, chemo-informatics, and discrete and stochastic methods for bioinformatics.

KEYWORDS

Complex Networks Boolean Networks Neural Networks Chemical Graphs **Protein Informatics**





Recent Selected Publications

Melkman, A. A.; Guo, S.; Ching, W-K.; Liu, P.; Akutsu, T., On the Compressive Power of Boolean Threshold Autoencoders, IEEE Transactions on Neural Networks and Learning Systems, 34, 921-931 (2023).

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Cao, Y.; Pi, W.; Lin, C-Y.; Münzner, U.; Ohtomo, M.; Akutsu, T., Common Attractors in Multiple Boolean Networks, IEEE ACM Transactions on Computational Biology and Bioinformatics, 20, 2862-2873 (2023).

Tamura, T., Trimming Gene Deletion Strategies for Growth-Coupled Production in Constraint-Based Metabolic Networks: TrimGdel, IEEE ACM Transactions on Computational Biology and Bioinformatics, 20, 1540-1549 (2023).

On the Compressive Power of Autoencoders Using Linear Threshold Activation Functions

Artificial neural networks have recently been extensively applied to bioinformatics. Among various models of artificial neural networks, autoencoders attract much attention because of their power to generate new objects such as protein sequences and chemical structures. An autoencoder is a layered neural network (Figure 1) consisting of an encoder which compresses an input vector to a lower dimensional vector, and a decoder which transforms the lowdimensional vector back to the original input vector (or one that is very similar). Although it is often mentioned that autoencoders perform dimensionality reduction, a kind of data compression, how data are compressed is not yet very clear. Therefore, we study the numbers of nodes and layers that are required to ensure that each vector in a given set of distinct input binary vectors is transformed back to its original using a autoencoder model with linear threshold activation functions. We show that for any set of distinct vectors there exists a seven-layer autoencoder with the optimal compression ratio, but that there is a set of vectors for which there is no three-layer autoencoder with a middle layer of the same size. We also study the numbers of nodes and layers required only for encoding, and the results suggest that decoding is more difficult than encoding.

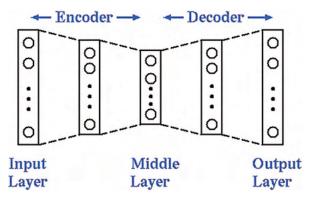
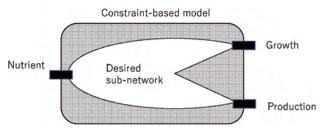


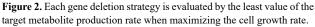
Figure 1. Architecture of an autoencoder.

Trimming Gene Deletion Strategies for Growth-Coupled Production in Constraint-Based Metabolic Networks: TrimGdel

When simulating genome-scale metabolite production using constraint-based metabolic networks, it is often necessary to find gene deletion strategies which lead to growth-coupled production, which means that target metabolites are produced when cell growth is maximized. One of the best current methods for this problem is the minimal cut set-based method, which utilizes the fact that minimal cut sets in the primal network are the elementary modes in the corresponding dual network. This method is effective when the number of gene deletions is relatively small, but when the number of required gene deletions exceeds 20, the time required for the calculation is often unfeasible. Therefore, a complementing algorithm that is effective even when the required number of gene deletions is approximately 20 to 40 would be helpful because the number of genes that can be deleted in a strain is increasing with advances in genetic engineering technology. In this study, the present author developed an algorithm, TrimGdel, which first computes a strategy with many gene deletions that results in growth-coupled production and then gradually reduces the number of gene deletions while maintaining the production rate and growth rate. The results of the computer experiments showed that, for 34.2% of the target metabolites in iML1515, the genome-scale constraint-based model of Escherichia coli, TrimGel could calculate gene deletion strategies of size 40 or less (23.6% for between 21 and 40) leading to growth-coupled production. TrimGdel can calculate stoichiometrically feasible gene deletion strategies, especially of sizes 21 to 40, which lead to growth-coupled production of target metabolites, which include useful vitamins such as biotin and pantothenate, for which existing methods could not.

The developed software is available on https://github. com/MetNetComp/TrimGdel





Bioinformatics Center - Bio-knowledge Engineering -

https://www.bic.kyoto-u.ac.jp/pathway/index.html





Prof Senior Lect MAMITSUKA, Hiroshi NGUYEN, Hao Canh (D Sc) (D Knowledge Science)



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Program-Specific Res Distinguished Visiting Senior Lect PETSCHNER, Peter (Ph D)

Students

JIANG, Zhiqian (RS) OTAGIRI, Yuan (UG)

Guest Res Assoc

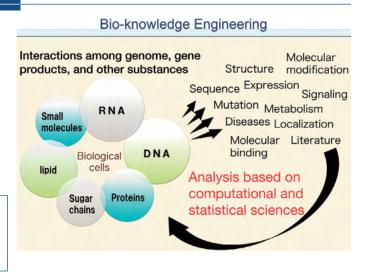
LI, Yufei Xi'an Jiaotong University, China, 2 May 2022–23 April 2023

Scope of Research

We are interested in graphs and networks in biology, chemistry, and medical sciences, including metabolic networks, protein-protein interactions and chemical compounds. We have developed original techniques in machine learning and data mining for analyzing these graphs and networks, occasionally combining with table-format datasets, such as gene expression and chemical properties. We have applied the techniques developed to real data to demonstrate the performance of the methods and find new scientific insights.

KEYWORDS

Bioinformatics	Machine Learning	
Data Mining	Artificial Intelligence	Systems Biology



Recent Selected Publications

Wang, X.; Sun, L.; Nguyen, C. H.; Mamitsuka. H., Multiplicative Sparse Tensor Factorization for Multi-View Multi-Task Learning, Proceedings of the 26th European Conference on Artificial Intelligence (ECAI 2023), 2560-2567 (2023).

Nguyen, D. A.; Nguyen, C. H.; Petschner, P.; Mamitsuka, H., SPARSE: A Sparse Hypergraph Neural Network for Learning Multiple Types of Latent Combinations to Accurately Predict Drug-drug Interactions, Bioinformatics (Proceedings of the 30th International Conference on Intelligent Systems for Molecular Biology (ISMB 2022)), 38 (Supplement 1), i333-i341 (2022).

You, R.; Qu, W.; Mamitsuka, H.; Zhu, S., DeepMHCII: A Novel Binding Core-Aware Deep Interaction Model for Accurate MHC II-peptide Binding Affinity Prediction, Bioinformatics (Proceedings of the 30th International Conference on Intelligent Systems for Molecular Biology (ISMB 2022)), 38 (Supplement 1), i220-i228 (2022).

Nguyen, C. H.; Mamitsuka, H., Learning on Hypergraphs with Sparsity, IEEE Transactions on Pattern Analysis and Machine Intelligence, 43(8), 2710-2722 (2021).

Nguyen, D. H.; Nguyen, C. H.; Mamitsuka, H., ADAPTIVE: leArning DAta-dePendenT, conclse molecular VEctors for fast, Accurate Metabolite Identification from Tandem Mass Spectra, Bioinformatics (Proceedings of the 27th International Conference on Intelligent Systems for Molecular Biology (ISMB/ECCB 2019)), 35(14), i164-i172 (2019).

Data Integrative Machine Learning: DIVERSE, An Example Approach to Personalized Medicine.

Multiple datasets can be found in any applications. For example, the main E-commerce data is a matrix of individuals (users) and items. Additionally, matrices on user demographic data and item contents can be obtained. In this case, the three matrices can be given, sharing the two dimensions, i.e. those of users and of items. Our focus is personalized medicine, where the main data is a matrix of individuals (patients, eventually cell lines) and their drug responses. The problem to be addressed is the drug response prediction, i.e. to predict unknown effective drugs for patients (cell lines). For this purpose, additional datasets can be used, such as a drug similarity matrix, drug-target interactions (a target is a protein, which is equivalent to the corresponding gene). These relevant data sources are called omics data, particularly in biology. Fig. 1 shows a schematic picture of omics data in drug response prediction, consisting of five matrices, including the main matrix R of drugs vs. cell lines.

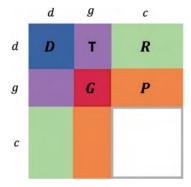


Figure 1. Conceptual integration configuration of the multiple data from three types of entities; d, g and c denote drugs, genes and cell lines, respectively.

Although large-scale omics data have been generated for drug response prediction, many machine learning methods have failed to achieve good performance for multiple heterogeneous data sources, because these methods have been designed for only a single type of data. Thus, a challenging task is to build precise prediction models on diverse data, coming from different sources, which are difficult to compare. In fact, data integration has to overcome several obvious problems, such as different data sizes, complexity, and noisiness. However, more importantly, dataintegrative machine learning methods need to decide which information is useful to be incorporated and how significant the information is for the prediction task. This is the most critical problem to be addressed for machine learning models with diverse multi-omics data. For this problem, we propose DIVERSE, a framework to efficiently integrate scientifically diverse data, i.e. genomic, chemical and molecular interaction information. DIVERSE has two unique features: 1) It is methodologically flexible. Most existing studies ignore uncertainty, and hence cannot accept missing values to predict missing drug responses of cancer cell lines. 2) It allows to compute importance weights over given multiple matrices, showing the contribution of the given matrices to prediction. DIVERSE solves these two practically important problems by using a Bayesian setting of matrix factorization. Fig. 2 shows the systematic framework of DIVERSE for the given matrix combination, shown in Fig. 1. In this framework, each dataset is incorporated into the matrix factorization framework of DIVERSE sequentially,

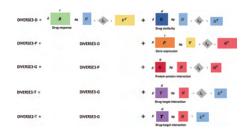


Figure 2. Overview of our systematic framework, DIVERSE, of integrating multiple data sets: importance weight tri-(or bi-)matrix factorization. We start with adding D to R (first row: DIVERSE3-D). We then add Pto DIVERSE3-D (second row: DIVERSE3-P). Similarly, we add G to DIVERSE3-P (third row: DIVERSE3-G) and T to DIVERSE3-G (fourth row: DIVERSE3-T). Another option of the last addition is bi-matrix factorization, and this is the last row: DIVERSE2-T.

We empirically validated the performance of DIVERSE, comparing with five other methods, including three state-of-the-art methods, under 5x5-fold cross-validation. Experimental results indicate that DIVERSE significantly outperformed all compared methods in both mean-squared error (MSE) and Spearman correlation coefficient (Sc), particularly for out-of-matrix prediction, which is a real-world setting and much harder than in-matrix prediction. Results clearly show the performance advantage of DIVERSE over the current methods for predicting drug responses. Table 1 shows one typical example of the results, where ten methods are compared.

	MSE 1. Std. Dev.	Se £ Std. Dev.
cls-mean	0.5227 ± 0.0027	-
all-mean	0.4181 ± 0.0726	-
MultiNMF	0.1581 ± 0.0721	0.1457 ± 0.0180
KRR	0.0764 ± 0.0125	0.2976 ± 0.0361
DrugCellNet	0.0455 ± 0.0044	-0.3423 ± 0.0259
DIVERSE3-D	0.0194 ± 0.0049	0.6750 ± 0.0186
DIVERSE3-P	0.0189 ± 0.0049	-0.6770 ± 0.0188
DIVERSE3-G	0.0186 ± 0.0035	0.6762 ± 0.0179
DIVERSE2-T	0.0185 ± 0.0040	0.6765 ± 0.0187
DIVERSE3-T	0.0183 ± 0.0033	0.6772 ± 0.0193

Table 1. MSE and Sc (average scores of 5x5 cross-validation) of ten compared methods in out-of-matrix prediction.

Furthermore, the results indicate that the MSE and Sc of DIVERSE were smoothly improved by the step-wise addition of each data set. Table 2 shows the performances of different data integration types of DIVERSE for three different cancer cell line datasets.

	CEDC101		Genetitabine		SN-38	
	MSE	Se	MSE	Sc	M51	Sc
DIVERSE3-D	0.(Ю0%6	0.916	0.00182	(1.930	0.00146	0.861
DIVERSE3-P	0.00099	0.910	0.00203	0.923	0.00122	0.884
DIVERSE3-G	0.40092	0.915	0.00211	0.919	0.00165	0.841
DIVERSE2-T	0.00087	0.922	0.00189	0.929	0.00119	0.894
DIVERSE3-IT	1 8000.0	0.926	0.00138	0.948	0.00121	0.887

Table 2. Average MSE and Spearman correlation scores over 5x5-fold cross-validation for three different types of cancer cell lines.

Finally, these advantages of DIVERSE were confirmed by several case studies. Overall, DIVERSE is useful for performing integrative machine learning for given multiple omics data sources, which has not been handled by a regular machine learning algorithm.

HAKUBI RESEARCHERS' ACTIVITIES IN ICR

Hakubi Project: Fosterage and Support of Young Researchers, Kyoto University

Research Topic

Program-Specific Assoc Prof TAHARA, Hirokazu (D Sc)

Outline of Research

Semiconductor nanostructures are attractive materials that provide a platform to enhance quantum effects. In nanomaterials, strongly-confined electrons and holes form unique quantum states such as multiexcitons, which are hardly generated in bulk semiconductors. Since multiexcitons consist of a few electrons and holes, their generation and dissociation processes have a great potential to increase electric signals in photon-to-current conversion. My research focuses on applications of quantum effects and control of photon-to-current conversion processes in semiconductor nanostructures. I will clarify the microscopic mechanism of photocarrier generation processes in coupled nanostructures and establish a way to recycle thermal and radiative energies.

Host Laboratory Laboratory of Nanophotonics

Optoelectronic Energy Recycling and Quantum Cooperative

Effects in Semiconductor Nanostructures

Host Professor KANEMITSU, Yoshihiko



iJURC Cooperative Research Subjects 2023

(1 April 2023 ~ 31 March 2024)

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STARTING-UP SUBJECTS

Development of Highly Active Metal Cluster Catalysts by Using (IN SPECIFIC FIELDS CHOSEN BY iJURC) Electron Transfer Network KONDO, Mio, Division of Applied Chemistry, Graduate School of Engineering, Osaka University Host in iJURC TANIFUJI, Kazuki Radiolysis of Concentrated Native Proteins by Accelerated Electrons RAFFY, Quentin, Institut Plurisdisciplinaire Hubert Curien (IPHC) Host in iJURC OGAWARA, Ryo Modulated Luminescence of Coordination Complex under Vibrational Strong Coupling Development of New Nano-Structure Target for ISOL HIRAI, Kenji, Research Institute for Electronic Science Hokkaido OHNISHI, Tetsuya, Nishina Center for Accelerator-Based Science, University RIKEN Host in iJURC KANEMITSU, Yoshihiko Host in iJURC WAKASUGI, Masanori Spectroscopic Study of Dot-in-Crystal Perovskites toward High-Pressure synthesis and Li Conducting Study of Li-Al-Cl Semiconductor Optical Refrigeration Compounds as Solid Electrolytes in Batteries YAMADA, Yasuhiro, Granduate School of Science, Chiba Uni-KOEDTRUAD, Anucha, Chinese Academy of Science (CAS), versitv Institute of High Energy Physics (IHEP), Chinese Spallation Host in iJURC KANEMITSU, Yoshihiko Neutron Source (CSNS) Host in iJURC SHIMAKAWA, Yuichi Quantum Properties of Lead Perovskite Solar Cells by Two-I Dimensional Optical Fourier Transform Spectroscopy Crystal Structures and Oxygen Conduction Properties Research OGAWA, Yoshihiro, Joetsu University of Education of Metal Oxides at High Temperature Host in iJURC KANEMITSU, Yoshihiko GUO, Haichuan, China Spallation Neutron Source Science Center (CSNS), Institute of High Energy Physics, Chinese Academy of Terahertz Laser by Topological Edge States in Non-Hermitian Sciences Systems Host in iJURC SHIMAKAWA, Yuichi OBUSE, Hideaki, Faculty of Engineering, Hokkaido University I Host in iJURC HIRORI, Hideki Development of Transformation of Lignin-Based Aromatic Building Blocks Using Organocatalyst Controlling Hydrogen Spillover on Oxides HASHIMOTO, Toru, Department of Applied Chemistry, Faculty HOSOKAWA, Saburo, Faculty of Materials Science and Engineerof Engineering, Sanyo-Onoda City University ing, Kyoto Institute of Technology Host in iJURC NAKAMURA, Masaharu Host in iJURC KAN, Daisuke Ι Synthesis of Phosphine-Protected Iron Clusters to Study Their Development of Defective Nickel Oxide Catalysts for Highly Magnetic Properties Selective Functionalization SHIGA, Takuya, Department of Chemistry, Institute of Pure and TAKETOSHI, Ayako, Faculty of Engeneering, Yokohama National Applied Sciences, University of Tsukuba University Host in iJURC HIGAKI, Tatsuya Host in iJURC NAKAMURA, Masaharu Catalytic Activation of Silicon-Oxygen Bond via Nucleophilic Efficient Synthesis and Physical Properties of *π*-Extended Activation of Silane Molecules Bearing Difluoroboryl or Sulfonyl Groups KAMEO, Hajime, Department of Chemistry, Graduate School of MITSUDO, Koichi, Graduate School of Natural Science and Science, Osaka Metropolitan University Technology, Okayama University Host in iJURC OHKI, Yasuhiro Host in iJURC WAKAMIYA, Atsushi Asymmetric Synthesis of Planar-Chiral Metallocenes by Plane-to-A Study on Statistical Machine Learning for Efficient Graph Plane Chirality Transfer Structured Data Analysis OGASAWARA, Masamichi, Department of Natural Science, KARASUYAMA, Masayuki, Department of Computer Science, Nagoya Institute of Technology Graduate School of Science and Technology, and Research Cluster on "Functional Material Development for Agro-/Medo-/ Host in iJURC MAMITSUKA, Hiroshi Pharmachemicals", and Tokushima International Science Institute, Tokushima University Evaluation of Prediction with MetNetComp Using Tensor Host in iJURC OHKI, Yasuhiro Decomposition Based Unsupervised Feature Extraction TAGUCHI, Yoshihiro, Faculty of Science and Engineering, Chou Carbon Fixation Catalysts Composed of Well-Defined Cu-Hydride University Host in iJURC TAMURA, Takeyuki Complexes and Functionalized Organosilica NAKAJIMA, Takayuki, Department of Chemistry, Faculty of Science, Nara Women's University Control and Analysis of Complex Networks via Probabilistic Host in iJURC OHKI, Yasuhiro Minimum Dominating Sets NACHER, Jose, Department of Information Science, Faculty of Science, Toho University Host in iJURC AKUTSU, Tatsuya

I: International Joint Research

F: Female PI

Elucidation of Host-Giant Virus Interaction Using Transcriptomics of Giant Virus-Infected Acanthamoeba Cells

TAKEMURA, Masaharu, Institute of Arts and Sciences, Kagurazaka Division, Tokyo University of Science

Host in iJURC OGATA, Hiroyuki

Development of a Viral Genome Information Infrastructure for Elucidation of Viral Dark Matter

NISHIMURA, Yosuke, JAMSTEC, Japan Agency for Marine-Earth Acience and Technology, Research Center for Bioscience and Nanoscience

Host in iJURC OGATA, Hiroyuki

Combining Tellurium Mediated Radical Polymerization and Multicomponent Polymerization towards Unique Stimuli Responsive Polypeptoids/poly(N-vinyl amide)s Copolymers DEBUIGNE, Antoine, Chemistry Department, Center for Education and Research on Macromolecules, University of Liege, Belgium Host in iJURC YAMAGO, Shigeru Ι

Studies of Geometric and Electronic Structure/Reactivity Correlation in Cofacial Metalloporphyrin Dimers OHTA, Takehiro, Department of Applied Chemistry, Faculty of Engineering, Sanyo-Onoda City University

Host in iJURC OHKI, Yasuhiro

Synthesis of Self-Assembled Azulene Derivatives Utilizing Boron, and Creation of New Reactions and Functions

WAKABAYASHI, Shigeharu, Department of Clinical Nutrition, Faculty of Health Science, Suzuka University of Medical Science Host in iJURC OHKI, Yasuhiro

Controlling of Secondary Structure in Polysiloxane Main Chain and Application for Chiral Silica HIRAI, Tomoyasu, Department of Applied Chemistry, Osaka

Institute of Technology

Host in iJURC TAKENAKA, Mikihito

Exploration of Novel Optical Phenomena in Semiconductors with High Quantum Efficiency of Radiation

KOJIMA, Kazunobu, Graduate School of Engineering, Osaka University

Host in iJURC KANEMITSU, Yoshihiko

Stoichiometry of Bioactive Trace Metals in the Osaka Bay and Its Inflowing River Waters

NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kindai University

Host in iJURC SOHRIN, Yoshiki

Study on High Selective Membrane Separation of Metal Ions by Use of Polimer Inclusion Membranes of Ionic Liquid Containing the Metal Complexes

MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education

Host in iJURC SOHRIN, Yoshiki

Fabrication and Characterization of Luminescent Thin Films of Lanthanide Complexes for Solid-State Ion Sensors

MIEDA, Eiko, Department of Chemistry, Graduate School of Science, Osaka Metropolitan University

Host in iJURC HASEGAWA, Takeshi F

Physicochemical Characterization of Novel Hybrid Partially Fluorinated Phospholipid Bilayers

SONOYAMA, Masashi, Faculty of Science and Technology, Gunma University

Host in iJURC HASEGAWA, Takeshi

Characterization of Molecular Orientation during Wear of Fluoropolymer

KASUYA, Motohiro, Faculty of Production Systems Engineering and Sciences, Komatsu University Host in iJURC HASEGAWA, Takeshi

Identification of Active Gibberellins in the Basal Land Plant Marchantia polymorpha

KOHCHI, Takayuki, Graduate School of Biostudies, Kyoto University

Host in iJURC YAMAGUCHI, Shinjiro

Preparation and Precise Characterization of Model Two-Dimensional Sheet-Shaped Polymers DOI, Yuya, Department of Materials Physics, Nagoya University Host in iJURC SATO, Takeshi

Spin Signals in a Ferrimagnetic Film near the Compensation Temperature

HIROHATA, Atsufumi, Nagoya University, Department of Materials Physics

Host in iJURC ONO, Teruo Ι

Study on the Spin Injection Using Perpendicularly Magnetized Ferromagnetic Conductor Film TANAKA, Masaaki, Nagoya Institute of Technology Host in iJURC ONO, Teruo

Demonstration of Topological Phase Control in Chalcogenide Superlattices

MOROTA, Misako, National Institute of Advanced Industrial Science and Technology (AIST) Host in iJURC ONO, Teruo F

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY iJURC)

Development of Energy Sensitive Muon Spin Rotation (muSR) Spectrometer MA, Yue, Meson Science Laboratory, RIKEN Host in iJURC TSUKADA, Kyo On the Mechanism of the CO₂ Reduction Catalyzed by Cubic [Mo₃S₄Pd] Clusters: a Computational Study SAMEERA, W. M. C., Department of Chemistry, University of Colombo Host in iJURC OHKI, Yasuhiro Ι

Development and Device Evaluation of New D-A Emitters Based on Rigidified Planar Triarylborone Acceptors MARDER, Todd B., Institut für Anorganische Chemie, Julius-Maximilians-Universität Würzburg Host in iJURC KAJI, Hironori Ι Design and Tailoring Advanced Functional Materials: Symmetry **Operation and High Pressure Synthesis** CHEN, Wei-Tin, Center for Condensed Matter Sciences, National Taiwan University Host in iJURC SHIMAKAWA, Yuichi Ι

High-Performance Materials for Energy Storage Electrochemical Devices

GARCIA MARTIN, Susana, Departamento de Química Inorgánica, Facultad de Ciencias Químicas, Universidad Complutense Host in iJURC SHIMAKAWA, Yuichi I F

Photocatalytic C-H Bond Functionalization ALAKANANDA, Hajra, Department of Chemistry, Visva-Bharat	
University Host in iJURC NAKAMURA, Masaharu	 RIBBE, Markus W., Chancellor's professor at Department of Molecular Biology and Biochemistry, Department of Chemistry, University of California, Irvine
Development of Unsymmetrical π -Electron Systems of Heavie	
Main Group Elements and Elucidation of Their Property WAMOTO, Takeaki, Department of Chemistry, Graduate Schoo of Science, Tohoku University	Radical-Polar Crossover Catalysis for Synthesis of Complex Natural Products
Host in iJURC MIZUHATA, Yoshiyuki	HAN, Sunkyu, Department of Chemistry, KAISTHost in iJURC OHMIYA, HirohisaI
Creation of Effective Oxidation Scavenger for Efficient Perovskite Based Solar Cells	- Development of Multi-Resonant TADF Emitters with Short
SASAMORI, Takahiro, Department of Chemistry, Faculty o Pure and Applied Sciences, University of Tsukuba	
Host in iJURC WAKAMIYA, Atsushi	
A Caging Strategy for Cholinergic Optopharmacology	_
ARAI, Satoshi, NanoLSI, Kanazawa University Host in iJURC OHMIYA, Hirohisa	Design and Synthesis of Linear Molecules for Improving Outcou- pling Efficiency of Solution-Possessed OLEDs RAJAMALLI, Pachaiyappan, Materials Research Centre, Indian
Development and Evaluation of THz-STM for Low-Temperature	e Institute of Science, Bangalore
and High Magnetic Field FACHIZAKI, Takehiro, School of Information Science and	
Fechnology, Tokai University Host in iJURC KANEMITSU, Yoshihiko	Precise Synthesis and Controlling Higher Order Structure of Tadpole-Like Janus Cellulose Nanocrystal
	GOTO, Atsushi, School of Physical & Mathematical Sciences -
Regioselective C-H Activation Enabled by Substrate Recognition ILIES, Laurean, Center for Sustainable Resource Science, RIKEN	
Host in iJURC NAKAMURA, Masaharu	Host in iJURC KINOSE, Yuji
Development of Co-Facial-Type Dinuclear Complexes	Development of Lead Free Metal Halide Perovskite
YAMAGUCHI, Yoshitaka, Faculty of Engeneering, Yokohama National University	a TACHIBANA, Yasuhiro, School of Engineering, PMT University Host in iJURC TERANISHI, Toshiharu
Host in iJURC NAKAMURA, Masaharu	
Developing Machine Learning Approaches for Prediction o	Synthesis of Graphene Nanoribbons Containing Non-Hexagonal f Rings
Protein Stability Changes upon Missense Mutations SONG, Jiangning, Biomedicine Discovery Institute, Monasl	
University Host in iJURC AKUTSU, Tatsuya	Host in iJURC HASHIKAWA, Yoshifumi
Host in iJURC AKUTSU, Tatsuya	Optoelectronic Materials with Open-Cage C ₆₀ Derivatives as
Learning to Develop Cancer Type Predictive Models	ZHANG, Sheng, Engineering Research Center for Nanomaterials
YANG, Jinn-Moon, Department of Biological Science and Technology, Institute of Bioinformatics & Systems Biology National Yang Ming Chiao Tung University	
Host in iJURC AKUTSU, Tatsuya] The Reactivity of Guanidino-Isatins in Prato Cycloaddition Reac- tion
Ecology and Evolution of Large and Giant DNA Viruses	MARGETIC, Davor, Laboratory for physical organic chemistry,
DELMONT, Tom O., CNRS/Genoscope/UMR8030 Host in iJURC OGATA, Hiroyuki	
Application of Metagenomics and a Temperature-Driven Mathe	Host in iJURC MURATA, Yasujiro
matical Model to Estimate the Global Distribution of Micromona Viruses	
DEMORY, David, CNRS, UMR723	SAEKI, Akinori, Department of Applied Chemistry, Graduate
Host in iJURC ENDO, Hisashi	School of Engineering, Osaka University Host in iJURC WAKAMIYA, Atsushi
Effective Biomolecular Analysis and Application to Medical and Agricultural Research	
Agricultural Research KAYANO, Mitsunori, Research Center for Global Agromedicine Obihiro University of Agriculture and Veterinary Medicine Host in iJURC MAMITSUKA, Hiroshi	
	Light-Driven Organosulfur Catalysis for Sugar Modification

HIRAI, Go, Graduate School of Pharmaceutical Sciences, Kyushu University Host in iJURC OHMIYA, Hirohisa

Synthesis of Polymers Having Carbazolophane Moiety and Their Application of Hole Transport and CPL Materials TANI, Keita, Osaka Kyoiku University Host in iJURC TSUJII, Yoshinobu

Elucidation of Design Principles of Covalent Organic Solid Solutions SUZUKI, Mitsuharu, Graduate School of Engineering, Osaka

University Host in iJURC MURATA, Yasujiro

Synthesis and Properties of Emissive Triplet Diradicals SHIMIZU, Akihiro, Graduate School of Engineering Science, Osaka University Host in iJURC HIROSE, Takashi

Polymerization of Functional Vinyltellurides Prepared by Flow Reactors

NAGAKI, Aiichiro, Faculty of Science, Hokkaido University Host in iJURC YAMAGO, Shigeru

Study on Dependence of Electron Delocalization on Charged, Spin and Excited States in Conjugated Macrocycles KISHI, Ryohei, Graduate School of Engineering Science, Osaka University

Host in iJURC KAYAHARA, Eiichi

A Study on Radicals in Macrocyclic Systems: SOMO-HOMO Energy Conversion

ABE, Manabu, Graduate School of Advanced Science and Engineering, Hiroshima University

Host in iJURC KAYAHARA, Eiichi

Synthesis and Functionally Development of Donor-Acceptor Cycloparaphenylene Derivatives through Reorganization of Macrocyclic Gold Complexes via Dynamic Gold-Carbon Bonds TSUCHIDO, Yoshitaka, Faculty of Science Division I, Tokyo University of Science

Host in iJURC KAYAHARA, Eiichi

Trace Metal Elemental and Isotopic Composition in the North Pacific Ocean: Sources and Internal Cycling (4)

HO, Tung-Yuan, Research Center for Environmental Changes, Academia Sinica

Host in iJURC SOHRIN, Yoshiki Ι

Resolving the Structure-Dynamics-Property Relationship in Polymer Nanocomposites under Uniaxial Stretching-III

KOGA, Tadanori, Department of Material Science and Chemical Engineering, Stony Brook University

Host in iJURC TAKENAKA, Mikihito Ι

High Frequency Response of Polymeric Liquids: Rheology and **Dielectric Relaxation**

SUKUMARAN, Sathish K., Graduate School of Organic Materials Science, Yamagata University Ι

Host in iJURC SATO, Takeshi

Ultrafast Exciton Dynamics in Thermally Activated Delayed Fluorescence Molecular Aggregates with Heterogeneous Conformational Distribution

SOTOME, Hikaru, Division of Frontier Materials Science and Center for Promotion of Advanced Interdisciplinary Research, Graduate School of Engineering Science, Osaka University Host in iJURC KAJI, Hironori

Construction of Theoretical Guidelines for Designing Plasmonic Nanoallovs

IIDA, Kenji, School of Engineering, PMT University Host in iJURC TERANISHI, Toshiharu

Systems KIM, Kab-Jin, Department of Physics, Korea Advanced Institute of Science and Technology Host in iJURC ONO, Teruo Ι Non-Reciprocity of Spin Wave Propagation Generated by Orbital Hall Effect in Transition Metal Dichalcogenides KIM, Sanghoon, Department of Physics, University of Ulsan Host in iJURC ONO, Teruo Ι Research Toward Stable NV Centers at Shallow Region and Spin Dynamics in Diamond BALASUBRAMANIAN, Gopalakrishnan, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany Host in iJURC MIZUOCHI, Norikazu Ι Research on the Efficiency Enhancement of the NV Centers Creation in Nanodiamond SEGAWA, Takuya F, Laboratory for Physical Chemistry, ETH Zürich Host in iJURC MIZUOCHI, Norikazu I

Characterization of Quantum Magnon Using Hybrid Magnonic

Research toward High Sensitive NV Quantum Sensor in Diamond WRACHTRUP, Jörg, Stuttgart University Host in iJURC MIZUOCHI, Norikazu Ι

Development of Fe-Based D03 Type Alloys and Its Thermoelectric Property

NAGAHAMA, Taro, Hokkaido Univerisity Host in iJURC ONO, Teruo

Research of Surface State for Diamond Quantum Sensor TOKUDA, Norio, NanoMaterials Research Institute, KANAZAWA UNIVERSITY

Host in iJURC MIZUOCHI, Norikazu

Research of Quantum Technology and Diamond Synthesis for Higher Sensitivity of NV Quantum Sensor

MAKINO, Toshiharu, Advanced Power Electronics Research Center, The National Institute of Advanced Industrial Science and Technology

Host in iJURC MIZUOCHI, Norikazu

STARTING-UP SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Fabrication of Novel Cell Culture Substrates Using Well-Defined Porous Materials

YOSHIKAWA, Chiaki, National Institute for Materials Science (NIMS), Research Center for Functional Materials

Host in iJURC TSUJII, Yoshinobu I F

Synthesis and Characterization of Raw and Polymerized Asian Lacquer Samples: towards the Development of a Comprehensive Collection of Lacquer Reference Samples for Materials Science and Conservations Studies

BONADUCE, Ilaria, Department of Chemistry and Industrial Chemistry, University of Pisa

Host in iJURC	PINCELLA, Francesca	Ι	F	

Analysis of Novel Transporters for Strigolactones or Their Biosynthetic Intermediates

ZHAO, Yunde, Department of Cell and Developmental Biology, University of California San Diego

Host in iJURC MASHIGUCHI, Kiyoshi

Ι

Precise Synthesis and Viscoelastic Properties of Ring Polymers with High Purity and High Molecular Weight TAKANO, Atsushi, Department of Molecular and Macromolecular Chemistry, Nagoya University Host in iJURC MATSUMIYA, Yumi	Exploiting AtMYB60 Regulation for Water Use Efficiency and Drought Resistance in Crops GALBIATI, Massimo, National Council of Research (CNR), Institute of Agricultural Biology and Biotechnology (IBBA) Host in iJURC TSUGE, Tomohiko
Evaluation of Mechanical Properties for Polymer Elastomers with Pseudo-Rotaxane Type Cross-Links URAKAWA, Osamu, Department of Macromolecular Science, Osaka University Host in iJURC MATSUMIYA, Yumi	Chromatin, Epigenetic and Proteolytic Regulation of RNA Processing in Plant Morphogenesis RUBIO, Vicente, National Center of Biotechnology (CNB-CSIC), Plant Molecular Genetics Department Host in iJURC TSUGE, Tomohiko
Involvement of Phospholipids in Cytoplasmic Streaming in Plant Cells UEDA, Haruko, Osaka University, Department of Macromolecular Science Host in iJURC AOYAMA, Takashi	Self-Assembling Compounds That Selectively Inhibit Protein Phase-Separation ZHOU, Lu, School of Pharmacy, Fudan University Host in iJURC UESUGI, Motonari I Development of Cancer Vaccine Adjuvants with Optimized
Analysis of Membrane Lipid-Dependent Fermentation Stress Response in Acetic Acid Bacteria TOYOTAKE, Yosuke, Department of Biotechnology, Ritsumeikan University	Safety Profiles LI, Yan-Mei, Department of Chemistry, Tsinghua University Host in iJURC UESUGI, Motonari
Host in iJURC KURIHARA, Tatsuo Studies on the Structures and Functions of Two Alanine Dehy- drogenases in Geobacillus Kaustophilus OMORI, Taketo, Department of Biomedical Engineering, Osaka Institute of Technology	Red and Near-Infrared Multi-Resonance Thermally Activated Delayed Fluorescence Emitters BEDNAREK, Christin, Karlsruhe Institute of Technology, Institut of Organic Chemistry, IOC Host in iJURC KAJI, Hironori
Host in iJURC KURIHARA, Tatsuo Separation of Rare Earth Elements Using Solvent Impregnated Resin Using Surfactants KURAHASHI, Kensuke, Environmental and Materials Chemistry Course, Osaka Metropolitan University College of Technology	Construction of Heterologous Protein Secretion System at Low Temperatures by Using Cold-Adapted Microorganisms DAI, Xianzhu, College of Resources and Environment, Southwest University Host in iJURC KURIHARA, Tatsuo
Host in iJURC SOHRIN, Yoshiki Observation of Photothermal Conversion in 3D Quantum Dot Superlattices Using Pump-Probe Transient Absorption Spectros- copy	Structural and Functional Analysis of the Surface Polysaccharides of Outer Membrane Vesicles Released by Bacteria CORSARO, Maria Michela, Department of Chemical Sciences, University of Naples Federico II Host in iJURC KURIHARA, Tatsuo
GONOME, Hiroki, Graduate School of Science and Engineering, Yamagata University Host in iJURC SARUYAMA, Masaki Development of Cooperative Catalysis by Hybridization of	High Pressure Synthesis of the Metastable Rare-Earth Nickelates with Ni-Site Substitutions for Synchronizing Their Electronic Phase Transition and Potential Magnetic Transitions CHEN, Jikun, School of Materials Science and Engineering,
Supported Metal Nanoparticles with Metal Oxide Clusters YAMAZOE, Seiji, Graduate School of Science, Tokyo Metro- politan University Host in iJURC TERANISHI, Toshiharu	University of Science and Technology Beijing, RP China Host in iJURC SHIMAKAWA, Yuichi I Formation of Authigenic CaCO ₃ on the Ocean Floor below the
Study and Experiment of the High-Energy Electron Generation by the High-Power Laser-Irradiation to the Stacked CNT Target MATSUI, Ryutaro, Graduate School of Energy Science, Kyoto University	Compensation Depth CAI, Pinghe, Department of Marine Chemistry and Geochemistry, Xiamen University Host in iJURC SOHRIN, Yoshiki
Host in iJURC TOKITA, Shigeki	Fabrication of Nanotopographical Polymer Surfaces for Bacteri- cidal Properties-V ENDOH, Maya, Department of Material Science and Chemical
EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)	Engineering, Stony Brook University Host in iJURC TAKENAKA, Mikihito
Role of PIP5K Genes in Pollen Tube DevelopmentQU, Li-Jia, School of Life Sciences, Peking UniversityHost in iJURC AOYAMA, Takashi	Interdisciplinary Approach to Nanostructured Materials for Applications BUCHER, Jean-Pierre, Strasbourg Institute of Material Physics and Chemistry
Molecular Mechanisms of mRNA Processing Governing 3'UTR Ends by Using Plant as a Model System JARMOLOWSKI, Artur, Department of Gene Expression,	Host in iJURC TERANISHI, Toshiharu I Search for Four-Wave-Mixing in the Vacuum - Unveiling Dark
Adam Mickiewicz University, Institute of Molecular Biology and Biotechnology Host in iJURC TSUGE, Tomohiko	Components in the Universe - HOMMA, Kensuke, Graduate School of Advanced Science and Engineering, Hiroshima University Host in iJURC TOKITA, Shigeki

Advanced Oxygen - Mediated Flow Chemistry Electrochemical Control of Metal Oxides and Exploration of THOMAS, Wirth, School of Chemistry, Cardiff University Their Functional Properties Host in iJURC NAKAMURA, Masaharu TSUCHIYA, Takashi, International Center for Materials Nanoar-Ι chitectonics, National Institute for Materials Science Host in iJURC KAN, Daisuke Novel Strategy for Intracellular Delivery of Nanomedicines PUJALS, Sílvia, Institute for Advanced Chemistry of Catalonia Polymer-Brush-Decorated Hybrid Particles as Lubricant Additives (IQAC) Host in iJURC FUTAKI, Shiroh OHNO, Kohji, Osaka Metropolitan University I F Host in iJURC TSUJII, Yoshinobu Structural and Functional Analysis of Curvature-Inducing Eptides and Application Manipulation of Three Dimensional Structure of Polymer ULRICH, S. Anne, Karlsruhe Institute of Technology (KIT), Monoliths by 3D Printer Institute of Organic Chemistry (IOC) and Institute of Biological MURASE, Hitoki, Kyoritsu Women's University Interfaces (IBG-2) Host in iJURC TSUJII, Yoshinobu Host in iJURC FUTAKI, Shiroh I F Room Temperature Operable CdS/CdTe Type II Dimer-Quantum-Molecular Mechanisms for the Inactivation of a Growth Hormone dot Diode in Rice MAJIMA, Yutaka, Institute for innovative Research, Tokyo HE, Zuhua, Institute of Plant Physiology and Ecology, Chinese Institute of Technology Academy of Sciences Host in iJURC TERANISHI, Toshiharu Host in iJURC YAMAGUCHI, Shinjiro Ι Measurement of Quasi-Stable Strong Magnetic Field by the Inter-Cycloparaphenylenes and Chiral Fullerenes for Supramolecular action between a High-Power Laser and Structured Medium KISHIMOTO, Yasuaki, Graduate School of Energy Science, Architectures in Chiroptical Applications FUCHTER, Matthew J., Imperial College London (ICL), Kyoto University Host in iJURC TOKITA, Shigeki Chemistry Host in iJURC YAMAGO, Shigeru Ι Investigation of Cellular Uptake Mechanism Using Extracellular Chiral Cyclophenylene with an [2.2]Paracyclophane Core Vesicles BRÄSE, Stefan, Karlsruhe Institute of Technology, Institut of EGUCHI, Akiko, Department of Gastroenterology and Hepatology, Graduate School of Medicine, Mie University Biological and Chemical System, IBCS-FMS Host in iJURC YAMAGO, Shigeru Host in iJURC FUTAKI, Shiroh F Ι Development of Multi-Dimensional Perovskite Light-Emission Design of Intracellular Delivery Systems for Extracellular Vesicles and Photo-Response Materials NAKASE, Ikuhiko, Department of Biological Chemistry, Graduate LIN, Hao-Wu, Department of Materials Science and Engineering, School of Science, Osaka Metropolitan University National Tsing Hua University, Taiwan Host in iJURC FUTAKI, Shiroh Host in iJURC WAKAMIYA, Atsushi Ι Functional Analysis of Non-Canonical Strigolactones as Plant Correlation of Concentration and Orientation Fluctuations in Hormones and Root-Derived Signals Mixture of Liquid Crystal/Solvent Isotropic One-Phase State SETO, Yoshiya, School of Agriculture, Meiji University Host in iJURC YAMAGUCHI, Shinjiro SHIMADA, Ryoko, Department of Mathematics, Physics and Computer Science, Japan Women's University Host in iJURC SATO, Takeshi I F Development of Structurally Well-Defined Branched Supramolecular Polymers Real-Time Visualization of Cellular Phase-Separating Proteins HAINO, Takeharu, Graduate School of Advanced Science and KIKUCHI, Kazuya, Graduate School of Engineering, Osaka Engineering, Hiroshima University University Host in iJURC YAMAGO, Shigeru Host in iJURC UESUGI, Motonari SUBJECTS FOCUSING OF JOINT USAGE OF iJURC/ Remote Control of Cells by Synthetic Small Molecules NISHIKAWA, Makiya, Faculty of Pharmaceutical Sciences, **ICR FACILITIES** Tokyo University of Science Host in iJURC UESUGI, Motonari Microstructural Investigation by Atomic Resolution Transmission Electron Microscopy of Novel Alloys Investigation of Donor-Acceptor Molecular Systems by Quantum CHOMSAENG, Natthaphol, Advanced Materials Engineering, Chemical Calculations and Atomic-Scale Spectroscopy Burapha University KIMURA, Kensuke, Surface and Interface Science Laboratory, Host in iJURC HARUTA, Mitsutaka Ι RIKEN Host in iJURC KAJI, Hironori Electron Energy Loss Spectroscopy and High-Resolution Transmission Electron Microscopy of Novel Functional Materials Functional Analysis and Applications of Extracellular Vesicles CHAIRUANGSRI, Torranin, Industrial Chemistry, Chiang Mai Produced by Intestinal Bacteria University YAMASAKI, Shino, Department of Life Science and Biotech-Host in iJURC HARUTA, Mitsutaka Ι nology, Kansai University Host in iJURC KURIHARA, Tatsuo F

Plasmon Excitations in Charge-Density-Wave Systems: A Momentum-Dependent Electron-Energy Loss Spectroscopy Investigation

CHU, Ming-Wen, Center for Condensed Matter Sciences, National Taiwan University Ι

Host in iJURC HARUTA, Mitsutaka

High-Pressure Synthesis of Transition Metal Oxides with Novel Properties

JI, Kunlang, Centre for Science at Extreme Conditions and School of Chemistry, University of Edinburgh

Host in iJURC SHIMAKAWA, Yuichi Ι

Elucidation of Hydrogen and Helium Retention Behavior in **Fusion Materials**

MIYAMOTO, Mitsutaka, Interdisciplinary Faculty of Science and Engineering, Shimane University Host in iJURC HARUTA, Mitsutaka

Nano Structural Analysis of Cs4PbBr6/CsPbBr3 Composite for the Development of a Scintillator for Fast Electron Beam Detection

with High Efficiency SAITO, Hikaru, Institute for Materials Chemistry and Engineering, Kyushu University

Host in iJURC HARUTA, Mitsutaka

Optimization of Laser Irradiation Conditions for High-Quality Ion beam Generation by Laser-Driven Ion Acceleration KOJIMA, Sadaoki, Kansai Institute for Photon Science, National Institutes for Quantum Science and Technology Host in iJURC TOKITA, Shigeki

Mass Spectrometry Analysis for the Production of Advanced Chemical Materials from the Efficient Chemical Decomposition Process of Cedar Wood Tissue Structure

HATANO, Osamu, Faculty of Medicine, Nara Medical University Host in iJURC NAKAMURA, Masaharu

Theoretical Design of Low-Dimensional Silicon Material Embedded in a Flat Two-Dimensional Sheet and Exploration for **Operating Principles**

TAKAHASHI, Masae, Graduate School of Science, Tohoku University

Host in iJURC MIZUHATA, Yoshiyuki F

SUBJECTS ENCOURAGING JOINT PROGRAM

Determine the Three-Dimensional Structure of ¹³C=¹⁸O Labeled α-Synuclein(61-95) in the Langmuir-Blodgett Film and Supported Phospholipid Bilayer by MAIRS2

WANG, Chengshan, Department of Chemistry, Middle Tennessee State University

Host in iJURC HASEGAWA, Takeshi Ι

High-Efficacy Protein Chemical Synthesis

HOJO, Hironobu, Institute for Protein Research, Osaka University Host in iJURC FUTAKI, Shiroh Ι

Modulation of In-Cell Protein-Protein Interactions Using Mid-Sized Peptides

TAMAMURA, Hirokazu, Institute of Biomaterials and Bioengineering (IBB-TMDU), Tokyo Medical and Dental University Host in iJURC FUTAKI, Shiroh I

The 17th International Workshop for East Asian Young Rheologists

INOUE, Tadashi, Department of Macromolecular Science, Osaka University

Host in iJURC MATSUMIYA, Yumi Ι A novel Interdisciplinary Approach to Cancer Metabolism Research by Solid State Nuclear Magnetic Resonance Spectroscopy ITO, Takahiro, Institute for Life and Medical Sciences, Kyoto University

Host in iJURC KAJI, Hironori

iJURC Publications (Selected Examples)

Field-Free Superconducting Diode Effect in Noncentrosymmetric Superconductor/Ferromagnet Multilayers

Narita, H.; Ishizuka, J.; Kawarazaki, R.; Kan, D.; Shiota, Y.; Moriyama, T.; Shimakawa, Y.; Ognev, A. V.; Samardak, A. S.; Yanase, Y.; Ono, T., *Nat. Nanotechnol.*, **17**, 823-828 (2022). Abstract

The diode effect is fundamental to electronic devices and is widely used in rectifiers and a.c.-d.c. converters. At low temperatures, however, conventional semiconductor diodes possess a high resistivity, which yields energy loss and heating during operation. The superconducting diode effect (SDE), which relies on broken inversion symmetry in a superconductor, may mitigate this obstacle: in one direction, a zero-resistance supercurrent can flow through the diode, but for the opposite direction of current flow, the device enters the normal state with ohmic resistance. The application of a magnetic field can induce SDE in Nb/V/Ta superlattices with a polar structure, in superconducting devices with asymmetric patterning of pinning centres or in superconductor/ferromagnet hybrid devices with induced vortices. The need for an external magnetic field limits their practical application. Recently, a fieldfree SDE was observed in a NbSe2/Nb3Br8/NbSe2 junction; it originates from asymmetric Josephson tunnelling that is induced by the Nb₃Br₈ barrier and the associated NbSe₂/Nb₃Br₈ interfaces. Here, we present another implementation of zero-field SDE using noncentrosymmetric [Nb/V/Co/V/Ta]20 multilayers. The magnetic layers provide the necessary symmetry breaking, and we can tune the SDE by adjusting the structural parameters, such as the constituent elements, film thickness, stacking order and number of repetitions. We control the polarity of the SDE through the magnetization direction of the ferromagnetic layers. Artificially stacked structures, such as the one used in this work, are of particular interest as they are compatible with microfabrication techniques and can be integrated with devices such as Josephson junctions. Energy-loss-free SDEs as presented in this work may therefore enable novel non-volatile memories and logic circuits with ultralow power consumption.

Synergistic Surface Modification of Tin–Lead Perovskite Solar Cells

Hu, S.; Zhao, P.; Nakano, K.; Oliver, R. D. J.; Pascual, J.; Smith, J. A.; Yamada, T.; Truong, M. A.; Murdey, R.; Shioya, N.; Hasegawa, T.; Ehara, M.; Johnston, M. B.; Tajima, K.; Kanemitsu, Y.; Snaith, H. J.; Wakamiya, A., *Adv. Mater.*, **35**(9), 2208320 (2023). Abstract

Interfaces in thin-film photovoltaics play a pivotal role in determining device efficiency and longevity. In this work, the top surface treatment of mixed tin-lead (~1.26 eV) halide perovskite films for p-i-n solar cells is studied. Charge extraction is promoted by treating the perovskite surface with piperazine. This compound reacts with the organic cations at the perovskite surface, modifying the surface structure and tuning the interfacial energy level alignment. In addition, the combined treatment with C60 pyrrolidine tris-acid (CPTA) reduces hysteresis and leads to efficiencies up to 22.7%, with open-circuit voltage values reaching 0.90 V, \approx 92% of the radiative limit for the bandgap of this material. The modified cells also show superior stability, with unencapsulated cells retaining 96% of their initial efficiency after >2000 h of storage in N2 and encapsulated cells retaining 90% efficiency after >450 h of storage in air. Intriguingly, CPTA preferentially binds to Sn²⁺ sites at film surface over Pb²⁺ due to the energetically favored exposure of the former, according to first-principles calculations. This work provides new insights into the surface

chemistry of perovskite films in terms of their structural, electronic, and defect characteristics and this knowledge is used to fabricate state-of-the-art solar cells.

LiNbO₃-Type Polar Antiferromagnet InVO₃ Synthesized under High-Pressure Conditions

Tan, Z.; Lussier, J. A.; Yamada, T.; Xu, Y.; Saito, T.; Goto, M.; Kosugi, Y.; Vrublevskiy, D.; Kanemitsu, Y.; Bieringer, M.; Shimakawa, Y., *Angew. Chem. Int. Ed.*, **61(25)**, e202203669 (2022). Abstract

The ambient pressure cation disordered InVO₃ bixbyite has been predicted to form a GdFeO₃-type perovskite phase under high pressure and high temperature. Contrary to the expectation, InVO₃ was found to crystallize in the polar LiNbO₃-type structure with a calculated spontaneous polarization as large as 74 μ C cm⁻². Antiferromagnetic coupling of V³⁺ magnetic moments and a cooperative magnetic ground state below about 10 K coupled with a polar structure suggest an intriguing ground state of the novel LiNbO₃-type high-pressure InVO₃ structure.

Nitrogen Reduction by the Fe Sites of Synthetic $[Mo_3S_4Fe]$ Cubes

Ohki, Y.; Munakata, K.; Matsuoka, Y.; Hara, R.; Kachi, M.; Uchida, K.; Tada, M.; Cramer, R. E.; Sameera, W. M. C.; Takayama, T.; Sakai, Y.; Kuriyama, S.; Nishibayashi, Y.; Tanifuji, K., *Nature*, **607**, 86-90 (2022).

Abstract

 N_2 fixation by Nature is performed by nitrogenase, which employs a unique transition metal-sulfur-carbon cluster as its active-site cofactor ([(*R*-homocitrate)MoFe₇S₉C], FeMoco). Whereas synthetic counterparts of FeMoco, metal-sulfur clusters, have displayed binding of N_2 in a few examples, the reduction of N_2 by this class of compounds has been unknown. Here we show that the Fe atoms in our [Cp^R₃Mo₃S₄Fe] cubes (Cp^R = C₅Me₅, C₅Me₄SiMe₃, and C₅Me₄SiEt₃) capture an N_2 molecule and catalyze N_2 silylation to form N(SiMe₃)₃ under treatment with excess Na and Me₃SiCl. These results exemplify the first catalytic N_2 reduction by a synthetic metal-sulfur cluster with an Fe center supported only by S ligands. This work demonstrates the N_2 -reducing capability of Fe atoms in a S-rich environment, which Nature has selected to accomplish a similar purpose.

"Mamonoviridae", a Proposed New Family of the Phylum *Nucleocytoviricota*

Zhang, R.; Takemura, M.; Murata, K.; Ogata, H., Arch. Virol., **168**, 80 (2023).

Abstract*

Acanthamoeba castellanii medusavirus J1 is a giant virus that was isolated from a hot spring in Japan in 2019. Recently, a close relative of this virus, named medusavirus stheno T3, was isolated in Japan. Here, we describe their morphological, genomic, and gene content similarities and also propose to create a new family, "Mamonoviridae", a new genus, "Medusavirus", and two species, "Medusavirus medusae" and "Medusavirus sthenus", to classify these two viruses within the phylum Nucleocytoviricota.

*Permission to use this abstract was obtained from Springer Nature by Hiroyuki Ogata.

VISITING PROFESSORS' ACTIVITIES IN ICR



Vis Prof OOI, Takashi (D Sc)



Vis Prof TANAKA, Keiji (D Eng)



Vis Prof GARCIA MARTIN, Susana (Ph D)



Vis Assoc Prof SHINYA, Hikari (D Sc)

Vis Assoc Prof YASUHARA, Ryo (D Eng)



Laboratory of Synthetic Organic Chemistry

Professor, Nagoya University (Chikusa, Nagoya, Aichi 464-8601)

Lecture at ICR Toward Catalytic Control of Photo-induced Radical Reactions

Laboratory of Polymer Materials Science

Applied Chemistry, Kyushu University

Lecture at ICR

Interfaces

Chemistry

Distinguished Professor, Department of

(744 Motooka Nishi-ku, Fukuoka 819-0395)

Innovative Adhesion Technology Based

on 4-dimensional Multi-Scale Analysis of

Laboratory of Advanced Solid State

Professor, Department of Inorganic Chemistry,

(Plaza de las Ciencias Ciudad Universitaria

Recent Research Activities in Complutense

Project Associate Professor, Center for

Spintronics Research Network (CSRN), The

(7-3-1 Hongo, Bunkyo, Tokyo 113-8656)

First-Principles Studies on Spintronics

Laboratory of Laser Matter Interaction

Professor, National Institute for Fusion

(322-6 Oroshi-cho, Toki, Gifu 509-5292)

Research on Ultrafast Mid-Infrared Lasers

Using Fe-Doped Chalcogenide Crystals

Prof Em / Specially Appointed Prof

TOKITOH, Norihiro (D Sc)

Complutense University of Madrid

28040, Madrid, Spain)

University of Mardrid

University of Tokyo

Lecture at ICR

Materials

Science

Science

Lecture at ICR

Laboratory of Nanospintronics

Lecture at ICR



Vis Prof SODEOKA, Mikiko (D Pharm)



Vis Prof ISOBE, Hiroyuki (D Sc)



Vis Assoc Prof SAMEERA, W. M. C. (Ph D)



Vis Assoc Prof IMADA, Hiroshi (D Eng)



Vis Assoc Prof NATSUME, Yayoi



Laboratory of Bio-knowledge Engineering medical Innovation, Health and Nutrition

Project Leader, National Institutes of Bio-(7-6-8, Saito-Asagi, Ibaraki, Osaka 567-0085)

Lecture at ICR

Exploring Possible Drug-Target Molecules Based on Network Data-Driven Integrative Machine Learning

Prof Em / Specially Appointed Prof KANEHISA, Minoru (D Sc)

the Current Style

(Hongo, Bunkyo, Tokyo 113-0033)

Laboratory of Chemical Biology

Laboratory, RIKEN

University of Tokyo

Lecture at ICR

Lecture at ICR

kylation

Labeling

Chief Scientist, Synthetic Organic Chemistry

(2-1, Hirosawa, Wako, Saitama 351-0198)

1. Development of Bifunctional Fluoroal-

2. ReactionsTurn-ON Fluorescent Affinity

Laboratory of Synthetic Organotransformation

Professor, Department of Chemistry, The

2. Organic Chemistry: From Structure and Synthesis to Boundaries

1. Organic Chemistry: From the Basics to

Laboratory of Organometallic Chemistry

Associate Professor, Department of Chemistry, University of Colombo (00300, Colombo, Sri Lanka)

Lecture at ICR Introduction to Computational Chemistry

Laboratory of Molecular Materials Chemistry Senior Researcher, Surface and Interface

Science Laboratory, RIKEN (Wako, Saitama 351-0198)

Lecture at ICR

Depeloping Various Dimer Systems Based on Single-Molecule Manipulation Techniques and Evaluation of Their Optical Properties



Retirement

Professor AOYAMA, Takashi Division of Biochemistry – Molecular Biology –

On March 31st, 2024, Dr. Takashi Aoyama retired from Kyoto University after 39 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Aoyama was born in Osaka Prefecture on November 7th, 1958. He graduated from the Faculty of Science, Kyoto University, majoring in Biological Sciences in 1981. He then proceeded to Graduate School of Science, Kyoto University, where he studied molecular mechanisms of gene expression regulation under the supervision of late Professor Mitsuru Takanami. In 1985, he left Graduate School to be appointed as Research Associate at Institute for Chemical Research, Kyoto University. In 1988, he was appointed Assistant Professor of Institute for Chemical Research, Kyoto University, and promoted to Associate Professor in 1994, and to Professor in 2009, directing the Laboratory of Molecular Biology. In 1987, he was granted a doctoral degree with the thesis entitled "Essential structure of E. coli promoter". On leave from the University during 1991 to 1993, he joined the Laboratory of Plant Molecular Biology, directed by Professor Nam-Hai Chua at The Rockefeller University.

Dr. Aoyama devoted himself in understanding the molecular function regulating gene transcription. His research started from studying the basic structure sequence elements determining the promoter function in Escherichia coli. Then he elucidated the gene expression control mechanism for T-DNA transfer and its integration into a plant nuclear genome from Agrobacterium rhizogenes and A. tumefaciens species. During his stay at The Rockefeller University, he development a novel chemical induction system for transcription in plants, utilizing the regulatory mechanism of vertebrate steroid hormone receptors. He developed a chimeric transcription factor that combined the receptor domain of the mammalian glucocorticoid receptor GR, the transcription activation domain of the herpesvirus transcription factor VP16, and the DNA binding domain of the Saccharomyces cerevisiae transcription factor GAL4. By expressing this chimeric transcription factor GVG in transformed plants, he established a chemical transcription induction system that effectively works in individual plants, for the first time. Today, this novel system is openly used in basic research and is applied in the commercial research field through licensed patents.



His investigation of the transcriptional control network in plant cell morphogenesis, and the following elucidation of the regulation in plant lipid signaling, were all founded on his unique style of research utilizing reverse genetic methods and plant transformants. He took advantage of the chemically induced reverse genetic methods to investigate the downstream of the transcription factor GL2, which plays a central role in the formation of single-celled trichomes and root hairs. He designed an extensive gene search strategy using the model plant Arabidopsis thaliana, and identified genes encoding the lipid metabolic enzyme PLDC1 and genes encoding bHLH-type transcription factors as direct target genes. Achievements on PLDC1 were published in the Science journal in 2003 and was featured on the cover page, as important evidence showing the involvement of lipid signaling in plant cell morphogenesis.

He then expanded his research interests to the role of lipid signals in plant cell morphogenesis, and analyzed the biological functions of PLD and PIP5K. Studies using root hair cells and pollen, as a model for single cell morphogenesis, revealed that PIP5K and its product $PI(4,5)P_2$ play a central role together with small G proteins in establishing and maintaining intracellular polarity. In addition to this, the research of analyzing the loss of function mutants of the nine major PIP5K genes of Arabidopsis and their multiple mutants have been internationally recognized as diligent, outstanding, field-leading work, to the complete the serial elucidation of the role of $PI(4,5)P_2$ signals in plants.

He has been invited to give keynote lectures at numerous international conferences. His achievements have been published in 70 original academic papers in international journals, 15 reviews and commentaries, and 11 co-authored books. He has also contributed to the field of plant science, serving as the secretary-general of the Japanese Society of Plant Physiologists and on the editorial board of the international journal, Plant Cell and Physiology.

Throughout his career, he enlightened many followers not only at Kyoto University but also at other universities and institutes with his thoughtful character. His contribution to Kyoto University and the Institute for Chemical Research through his scientific, educational, and administrative activities is hereby greatly acknowledged.

Retirement

Professor KANEMITSU, Yoshihiko International Research Center of Elements Science – Nanophotonics –

On March 31st 2024, Professor Yoshihiko Kanemitsu retired from Kyoto University and was honored with the title of Professor Emeritus of Kyoto University. Dr. Kanemitsu joined the Institute for Chemical Research in 2004 as a professor of physics. He set up a new laboratory for semiconductor physics and optical materials science as part of the International Research Center of Elements Science.

Throughout his academic career, Professor Kanemitsu has explored unique optical and electronic properties of semiconductors by applying various laser spectroscopic techniques. Semiconductor bulk crystals and nanomaterials are widely used in solar cells, light-emitting diodes, lasers, and other optoelectronic devices. His fundamental work has contributed to our basic understanding of semiconductor photophysics, helped improve the performance of optoelectronic devices, and led to the development of new concepts in optoelectronics. His outstanding achievements center on the exciton physics of semiconductor nanomaterials and the photophysics of perovskite-type semiconductors.

Professor Kanemitsu developed space- and time-resolved laser spectroscopy apparatus and methods for the study of optical properties of semiconductor quantum structures, including single-dot spectroscopy, photon correlation spectroscopy, and femtosecond transient absorption spectroscopy. He studied the luminescence spectra of isolated carbon nanotubes and single nanocrystals at low temperatures and elucidated their complicated excited state structures. He also clarified the important role of excitons, trions, and biexcitons in governing the luminescence spectra of carbon nanotubes and nanocrystals. In addition, he discovered the coherent state of multiple excitons in nanocrystals, as well as high-order harmonic light emission from nanocrystals. These findings highlight the importance of precise control of the exciton dynamics and exciton complexes for improving the performance of nanomaterial-based photonic devices. He also presented new device concepts based on nanomaterials with high-efficiency nonlinear optical response.

Professor Kanemitsu has also contributed extensively to the area of metal-halide perovskite semiconductors. After showing that halide perovskites are direct-gap semiconductors, he confirmed that the efficient luminescence is due



to free carrier band-to-band recombination. He also discovered the phenomena of efficient photon recycling in thick perovskite single crystals. These seminal studies explained the reasons why halide perovskites are such excellent materials for solar cells. Along the way, he explored unique nonlinear optical phenomena such as high-order harmonic light emission, the Autler-Townes effect, and negative thermo-optic coefficients in these materials. His pioneering works in this area opened a new avenue of semiconductor optics and optoelectronic applications.

As a leading scientist in his field, Professor Kanemitsu has many other accomplishments. He served as the chairman of the 125 Committee on Mutual Conversion between Light and Electricity, The Japan Society of the Promotion of Science, and as an R&D management committee member of the ALCA and MIRAI programs, Japan Science and Technology Agency. He is also a member of several advisory committees of international conferences for optical spectroscopy of condensed matter. He established the Endowed Research Section at the Institute for Chemical Research supported by the Sumitomo Electric Group CGR Foundation.

Throughout his career, Professor Kanemitsu has published over 400 papers and presented many invited talks at international conferences and meetings. His achievements have been internationally recognized, and he has received many awards and prizes including the Marubun Research Encouragement Award (1998), Phosphor Award (2004), The Ichimura Prize in Science for Distinguished Achievement (2005), The Inoue Prize for Science (2006), The Yazaki Science Award (2006), The Eto-Hosoya Prize (2018), The Shimadzu Prize (2019), The Kato Memorial Award (2019), The Ichimura Prize for Science against Global Warming for Distinguished Achievement (2021), American Physical Society Outstanding Referee (2022), and The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology (2022). In 2023 he was made a fellow of the Japanese Society for Applied Physics.

His contribution to Kyoto University through his scientific, educational, and administrative activities is acknowledged. His warm and sincere personality will remain deep in the hearts of his colleagues and students.

Awards

TAMAO, Kohei

Order of Culture Cabinet Office, Government of Japan



3 November 2023



Highly Cited Researcher 2023 Clarivate



TOKITOH, Norihiro



The 10th Japan Physical Organic Chemistry Award

"Challenging Research toward the Creation of Unexplored Molecules of Heavier Main Group Elements"

The Society of Physical Organic Chemistry, Japan

14 September 2023

NAGAO, Kazunori



The Young Scholar Lectures of the Chemical Society of Japan

"Carbocation Generation through Light-Driven Radical-Polar Crossover and the Application to Bond Formation Reaction"

The Chemical Society of Japan

22 March 2023





Nanoscale Horizons Award

The 21st Annual Meeting of the Society of Nanoscience and Technology

"Structural Control of Three-Dimensional Nanocrystal Superlattice"

The Society of Nano Science and Technology

13 May 2023

Young Scientist Award

Division of Colloid and Surface Chemistry

"Exploration of Diverse Nanomaterials Based on the Precise Chemical Synthesis of Inorganic Nanocrystals"

The Chemical Society of Japan

12 September 2023







Oral Presentation Award for Young Scientist

The 74th Divisional Meeting of Division of Colloid and Surface Chemistry

"Synthesis of 3D Ag Nanoparticle Superlattices and Their Structure-Specific Functions"

The Chemical Society of Japan

31 October 2023



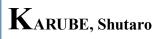


Young Scientist Award of the Physical Society of Japan, 2023

"Study of Coherence in Solid Materials and its Exploitation for Quantum Sensing"

The Physical Society of Japan

23 March 2023





The Japan Institute of Metals and Materials Young Researcher Award

"Creation of Novel Spin-Orbit Materials and Research on the Principle of Spin Current Generation"

The Japan Institute of Metals and Materials

20 September 2023

NARITA, Hideki



Young Scientist Research Award

The 14th JSAP Superconductors Division

"Field-Free Superconducting Diode Effect in Noncentrosymmetric Superconductor/Ferromagnet Multilayers"

JSAP Superconductors Division

15 March 2023

HTSF Young Scientist Research Award

The 6th High Temperature Superconductivity Forum

"Field-Free Superconducting Diode Effect in Superconductor/ Ferromagnet Multilayers"

High Temperature Superconductivity Forum

21 March 2023

2022 Tanaka Kikinzoku Memorial Foundation Young Researcher Award

"Control of Magnetic Superconductors Using Noble Metals and Development of Non-Volatile Superconducting Devices"

Tanaka Kikinzoku Memorial Foundation

31 March 2023

FUNADA, Shinsaku



The 54th JSAP Young Scientist Presentation Award

The 70th JSAP Spring Meeting 2023

"Electrical Detection of Antiferromagnetic Dynamics in GdCo Thin Films by Using a 154 GHz Gyrotron Irradiation"

The Japan Society of Applied Physics

19 September 2023

TAGA, Kotaro



Student Presentation Award of the Physical Society of Japan (Division 3)

JPS 78th Annual Meeting

"Frequency and Magnetic Field Angle Dependence of the Coupling between Spin Wave and Surface Acoustic Wave in NiFe Thin Film"

The Physical Society of Japan

14 October 2023

IMANISHI, Miki



The 28th SJWS Award

"Development of an Enzymatic Detection Method for RNA Methylation and Its Application"

The Society of Japanese Women Scientists

28 May 2023

KURIYAMA, Masashi



Best Presentation Award for Young Scientists

The 96th Annual Meeting of the Japanese Biochemical Society

"Correlation Analysis Between Peptide-mediated Intracellular Delivery Efficiency and Gene Expression"

The Japanese Biochemical Society

31 October 2023

MICHIBATA, Junya



The Best Student Presentation Award (Oral)

The 143rd Annual Meeting of the Pharmaceutical Society of Japan

"Liquid-Liquid Phase Separation Formation by Macromolecule Delivery Peptides Bearing Polysaccharides and its Application for Cytosolic Antibody Delivery"

The Pharmaceutical Society of Japan

Best Presentation Award

25 April 2023

The 24th Symposium on Drug Interactions with Biological Membranes

"Microparticle Formation by Macromolecule Delivering Peptides Bearing Polysaccharides and its Application for Cytosolic Antibody Delivery"

Division of Physical Sciences, The Pharmaceutical Society of Japan

20 October 2023

NAKAGAWA, Yuna



Excellent Presentation Award

The 2022 Master's Thesis Presentation at Graduate School of Pharmaceutical Sciences, Kyoto University

"Intracellular Delivery of Extracellular Vesicles Using Macropinocytosis-Inducing Peptide"

Graduate School of Pharmaceutical Sciences, Kyoto University

24 March 2023

Best Presentation Award

The 24th Symposium on Drug Interactions with Biological Membranes

"Improvement of the Membrane Fusion of Extracellular Vesicles by Loading SARS-CoV-2 Spike Proteins"

Division of Physical Sciences, The Pharmaceutical Society of Japan

20 October 2023

OTONARI, Kenko



Chairman's Special Award

The 24th Annual Meeting of the RNA Society of Japan

"Development of Higher Sequence-Selective and Timing-Controlled m6A Demethylation Tool"

RNA Japan

7 July 2023

Best Presentation Award for Young Scientists

The 96th Annual Meeting of the Japanese Biochemical Society

"Creation of Higher Sequence-Selective and Timing-Controlled m6A Demethylation Tool"

The Japanese Biochemical Society

31 October 2023

ТОН, Kohei



ICR Award for Graduate Students

"Chemoproteomic Identification of Blue-Light-Damaged Proteins"

Institute for Chemical Research, Kyoto University

1 December 2023

SATO, Hiroki



The 54th JSAP Young Scientist Presentation Award

The 70th JSAP Spring Meeting 2023

"Analysis of Charge Traps in Organic Amorphous Film by Multiscale Simulation"

The Japan Society of Applied Physics

19 September 2023

TAKANO, Shotaro



The Okada Prize

The 2023 Fall Meeting of the Oceanographic Society of Japan

"Development of an Analytical Method for Trace Metal Isotopes and Its Application to Marine Chemistry"

The Oceanographic Society of Japan

1 April 2023

The Japan Society for Analytical Chemistry Award for Younger Researchers, 2023

The 72nd Annual Meeting of the Japan Society for Analytical Chemistry

"Isotopic Analysis of Trace Metals for Geochemistry and Marine Chemistry"

The Japan Society for Analytical Chemistry

14 September 2023

ZHENG, Linjie



Young Scientist Award

The 119th meeting of the Japan Society for Plasma Spectrochemistry

"Establishment of a Simultaneous Analysis for Nine Trace Metals (Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb) in Seawater and Elucidation of their Sectional Distribution in the Pacific Ocean"

The Japan Society for PLASMA Spectrochemistry

12 May 2023

HASEGAWA, Takeshi



Academic Award

"Development of Multiple-Angle Incidence Resolution Spectrometry and its Applications in Thin Film Science" The Spectroscopical Society of Japan

5 October 2023

ZHU, Mengshan



Young Presentation Award

The 96th Annual Meeting of the Japanese Biochemical Society

"A Predicted Glycosyl Transferase Plays a Crucial Role in the Biogenesis of Extracelluar Membrane Uesicles of *Shewanella vesiculosa* HM13"

The Japanese Biochemical Society

31 October 2023

NAKAMURA, Tomoya



NIPPON SHOKUBAI Award in Synthetic Organic Chemistry

"Development of Monolayer Electron-Collecting Materials for Efficient Lead-Free Perovskite Solar Cells"

The Society of Synthetic Organic Chemistry, Japan (SSOCJ)

15 February 2023

The 12th Research Encouragement Award for Chemical Innovation

"Material Chemistry Approach for High-Performance Perovskite Tandem Solar Cells"

Japan Association for Chemical Innovation (JACI)

26 June 2023

TRUONG, Minh Anh

ICR Award for Young Scientists

"Tripodal Triazatruxene Derivative as a Face-on Oriented Hole-collecting Monolayer for Efficient and Stable Inverted Perovskite Solar Cells"

Institute for Chemical Research, Kyoto University

1 December 2023

HIRA, Shota

Innovative PV Encouragement Award

The 20th Next Generation Photovoltaic Power Generation System Symposium (1st Symposium of The Japan Photovltaic Society)

"Hole-Collecting Monolayer Materials based on Squaraine Structures for Perovskite Solar Cells"

The Japan Photovoltaic Society (JSES)

31 August 2023

TOKITA, Shigeki



"Development of Innovative Power Laser - Conduction-Cooled Active-Mirror Laser"

The Laser Society of Japan

31 May 2023

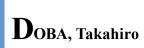
KIYOMURA, Tsutomu

Technical Support Contribution Award

The 22nd International Nanotechnology Exhibition & Conference

"Support for Fine-Structure Analysis by Transmission Electron Microscopy"

ARIM Japan





Inoue Research Award for Young Scientists

"Iron-Catalyzed C–H/C–H Coupling for Synthesis of Functional Small Molecules and Polymers"

Inoue Foundation for Science

14 December 2023





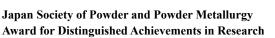
The Japanese Forest Society Student Award

"History of Policies Related to the Supply of Large Timber in Japanese National Forests"

The Japanese Forest Society

25 March 2023

SHIMAKAWA, Yuichi



"Synthesis of New Transition-Metal Oxides Showing Novel Properties"

Japan Society of Powder and Powder Metallurgy

6 June 2023

The Ceramic Society of Japan Awards for Academic Achievements in Ceramic Science and Technology

"Discovery of Novel Functionalities in Charge-Transition Oxides"

The Ceramic Society of Japan

7 June 2023





OHKI, Yasuhiro



The Chemical Society of Japan Award for Creative Work

The 103rd CSJ Annual Meeting

"Synthesis of Biomimetic Cluster Complexes and Reduction of Inert Small Molecules"

The Chemical Society of Japan

23 March 2023

KANEMITSU, Yoshihiko



The 17th JSAP Fellow (2023)

"Pioneering Research on Nano-Semiconductor Photophysics and Photonics"

The Japan Society Applied Physics



YUMOTO, Go



Paper Presentation Encouragement Award

The 43rd Annual Meeting of the Laser Society of Japan

"Development of Polarization-Resolved Pump-Probe Microscopy and Observation of Ultrafast Two-Dimensional Exciton Spin Transport"

The Laser Society of Japan

31 May 2023

SEKIGUCHI, Fumiya



Excellent Paper Presentation Award

The 43rd Annual Meeting of the Laser Society of Japan

"Polarization Anomaly of High Harmonics Generated from a Solid Reflecting the Crystal Symmetry and Non-Perturbative Nonlinear Dynamics"

The Laser Society of Japan

31 May 2023





ICR Award for Graduate Students

"Exciton-Phonon and Trion-Phonon Couplings Revealed by Photoluminescence Spectroscopy of Single CsPbBr₃ Perovskite Nanocrystals"

Institute for Chemical Research, Kyoto University

1 December 2023





Paper Presentation Encouragement Award

The 43rd Annual Meeting of The Laser Society of Japan

"Controlling High-Order Harmonic Generation Using Quantum Confinement Effects of Semiconductor Nanocrystals"

The Laser Society of Japan

31 May 2023

ZHANG, Zhenya

ICR Award for Graduate Students

"Generation of Third-Harmonic Spin Oscillation from Strong Spin Precession Induced by Terahertz Magnetic near Fields"

Institute for Chemical Research, Kyoto University

1 December 2023

SAKAMOTO, Minoru

Student Presentation Award of the Physical Society of Japan (Division 5)

2023 Spring Meeting of the Physical Society of Japan

"Controlling High Harmonic Generation in GaAs by Excitation Polarization: Enhancement of Harmonic Yields and Emergence of Nonlinear Optical Activity"

The Physical Society of Japan

31 March 2023

DAIKOKU, Yusuke



Student Presentation Award of the Physical Society of Japan (Division 5)

2023 Annual Meeting of the Physical Society of Japan

"Light-Induced Phase Separation in ABX₃-Type Perovskite Semiconductors Studied by Hyperspectral Imaging"

The Physical Society of Japan

14 October 2023

ENDO, Hisashi



Oceanochemistry Encouragement Prize

"Study on Marine Biogeochemical Cycles Using the Molecular Biological Techniques"

RIOC, Research Institute for Oceanochemistry Foundation

22 April 2023



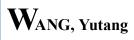


ICR Award for Young Scientists

"Mirusviruses Link Herpesviruses to Giant Viruses" Institute for Chemical Research, Kyoto University

1 December 2023

Poster Awards





Best Poster Award

The 57th Meeting for Young Scientists on Organic Reactions

"Development of a New Germanium Atom Transfer Reagent"

Organizing Committee of the 57th Meeting for Young Scientists on Organic Reactions

12 August 2023

Тамамото, кеп



Excellent Presentation Award

The 31st Polymer Materials Forum

"Visualization and Understanding of Dynamic Wetting and Fluid Behavior at the Polymer Brush Interface"

The Society of Polymer Science, Japan

25 May 2023

IPC2023 Poster Award: Langmuir Award

The 13rd SPSJ International Polymer Conference (IPC2023)

"Hydration and Anti-Icing Properties of Hydrophilic Concentrated Polymer Brushes"

The Society of Polymer Science, Japan

21 July 2023

HU, Weizhe



Poster Award

The 33rd Symposium on Physical Organic Chemistry

"Circularly Polarized Luminescence Properties of Dibenzo[7] helicenes and Single Crystal Structures Depending on the Position of Benzo Annulation"

The Society of Physical Organic Chemistry, Japan

14 September 2023

BCSJ Award for Poster Presentation

The 2nd Seminar on International Core-to-Core Project on Nano Carbon Device Science at Kyoto

"Non-Linear Molecular Spring Properties of a Dibenzo[c,u][7] helicene Derivative Derived from Intramolecular Non-Covalent Interactions"

Bulletin of the Chemical Society of Japan

6 October 2023

JIANG, Yuhan



BCSJ Award for Poster Presentation

The 10th Pacific Symposium on Radical Chemistry (PSRC-10)

"Synthesis of Topological Block Polymers by Organotellurium-Mediated Emulsion Polymerization in Water"

Organization Committee of the 10th Pacific Symposium on Radical Chemistry (PSRC-10)

9 June 2023

KAWASE, Riku



Poster Presentation Awards for Young Researchers

"Control of Impurity Incorporation into CVD Diamond toward Long Coherence Time of the NV Center by Optimizing Pressure"

Quantum Innovation 2023

5 December 2023

HARIKI, Nene

Best Poster Presentation Award

"Improving the Detection Efficiency of Nitrogen-Vacancy Center ODMR Signal in DNDs"

The Quantum Life Science Society



TOH, Kohei



Best Presentation Award

Drug Discovery Conference 2023 Yugawara

"Chemoproteomic Identification of Blue-Light-Damaged Proteins"

Division of Medicinal Chemistry, The Pharmaceutical Society of Japan

20 June 2023



19 May 2023

HAYASHI, Daiju

JSAP Poster Award

The 70th JSAP Spring Meeting 2023

"Observation of Mode Splitting by Magnon-Magnon Coupling in Synthetic Antiferromagnets"

The Japan Society of Applied Physics

10 May 2023

Poster Award

The 21st Annual Meeting of the Society of Nano Science and Technology

"Observation of Mode Splitting by Magnon-Magnon Coupling in Synthetic Antiferromagnets"

The Society of Nano Science and Technology

13 May 2023

KURIYAMA, Masashi



Excellent Poster Award

Interactive Seminar on Novel Medicinal Chemistry for Young Researchers (So-Yaku Konwa Kai)

"Identification of Biomolecules Involved in Intracellular Delivery of Biopolymers"

Division of Medicinal Chemistry, The Pharmaceutical Society of Japan

20 June 2023





Excellent Poster Prize

The 13th iCeMS Retreat

"Real-Time Monitoring of Biomolecular Condensates' States" WPI-iCeMS, Kyoto University

29 September 2023

SATO, Hiroki

Poster Prize

The 2nd International Research Center Seminar on Nanocarbon

"Molecular-Level Analysis of Charge Traps in An Organic Amorphous Film by Multiscale Simulation"

The Royal Society of Chemistry

6 October 2023

${f A}$ RAKI, Taisuke

Excellent Poster Award

The 46th Fluorine Conference of Japan

"Understanding of Physical Properties of Perfluoroalkanes by Infrared Spectroscopy Using Recrystallized Compounds"

The Society of Fluorine Chemistry, Japan

25 October 2023

SUGIMOTO, Emi

Student Poster Award

The 52nd Japan Conference on Crystal Growth

"Control of Crystal Orientation of Organic Semiconductors with Alkyl Side Chains by Low-Temperature Deposition"

The Japanese Association for Crystal Growth

25 December 2023

HIRA, Shota



Poster Award

The 33rd Symposium on Physical Organic Chemistry

"Hole-Collecting Monolayer Materials based on Squaraine Structures for Perovskite Solar Cells"

The Society of Physical Organic Chemistry, Japan

14 September 2023



Poster Award

The 50th Symposium. on Main Group Element Chemistry "Synthesis of Metal Halides Derivatives bearing Triptycyl Groups"

The Chemical Society of Japan (CSJ)

9 December 2023



IWASHIMIZU, Chisaki



Best Poster Award

Microscopy Conference 2023

"Different Image Contrasts between Atomic Resolution HAADF and EELS Mapping in Rutile TiO₂"

German Society for Electron Microscopy

2 March 2023

HARATA, Fuyuki



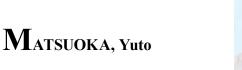
Poster Prize

The 5th Frontier Solar Cell Seminar

"Development of Fabrication Method for Large-Area Tin-Perovskite Thin Film"

The Executive Committee of the Frontier Solar Cell Seminar

15 December 2023



Best Poster Presentation Award in 69th Symposium on **Organometallic Chemistry**

The 69th Symposium on Organometallic Chemistry, Japan

"Difference in N_2 -Reducing Activity by $[Mo_3S_4M]$ (M = Fe, Co, Ni) Cubes"

Division of Organometallic Chemistry, The Kinki Chemical Society

27 September 2023

Publications International Research Collaborations Selected grants Theses

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY — Organoelement Chemistry —

Tajima, K.; Matsuo, K.; Yamada, H.; Fukui, N.; Shinokubo, H., Diazazethrene Bisimide: A Strongly Electron-Accepting π -System Synthesized *via* the Incorporation of Both Imide Substituents and Imine-Type Nitrogen Atoms into Zethrene, *Chem. Sci.*, **14(3)**, 635-642 (2023).

Hisa, T.; Kanno, Y.; Shirai, T.; Oshiki, T.; Mizuhata, Y.; Tokitoh, N.; Fukumoto, H.; Agou, T., Synthesis and Characterization of a Polystyrene-Type Polymer Bearing a Cyclic Perfluoroalkylene Group, *Polymer*, **265**, 125588 (2023).

Nagatomo, T.; Vats, A. K.; Matsuo, K.; Oyama, S.; Okamoto, N.; Suzuki, M.; Koganezawa, T.; Fuki, M.; Masuo, S.; Ohta, K.; Yamada, H.; Kobori, Y., Nonpolymer Organic Solar Cells: Microscopic Phonon Control to Suppress Nonradiative Voltage Loss via Charge-Separated State, *ACS Phys. Chem. Au*, **3(2)**, 207-221 (2023).

Suzuki, M.; Miura, M.; Ohkubo, E.; Karimata, H.; Aizawa, N.; Yamada, H.; Nakayama, K., Possibilities and Limitations in Monomer Combinations for Ternary Two-Dimensional Covalent Organic Frameworks, *J. Am. Chem. Soc.*, **145(5)**, 3008-3015 (2023).

Kurosaki, R.; Morimoto, H.; Matsuo, K.; Hayashi, H.; Yamada, H.; Aratani, N., An Atropisomerism Study of Large Cycloarylenes: [*n*]Cyclo-4,10-Pyrenylenes'Case, *Chem. Eur. J.*, **29(24)**, e202203848 (2023).

Igarashi, H.; Yamauchi, M.; Masuo, S., Correlation between Single-Photon Emission and Size of Cesium Lead Bromide Perovskite Nanocrystals, *J. Phys. Chem. A*, **14(9)**, 2441-2447 (2023).

Lv, X.; Morimoto, H.; Liu, N.; Kuzuhara, D.; Aratani, N.; Yamada, H.; Qiu, F.; Xue, S., Bent Dithienoporphyrin(2.1.2.1): Synthesis, Structure, Optical and Electronic Properties, and Metal Complexation, *J. Org. Chem.*, **88(6)**, 3466-3473 (2023).

Duan, Y.; Chen, M.; Hayashi, H.; Yamada, H.; Liu, X.; Zhang, L., Buckybowl and Its Chiral Hybrids Featuring Eight-Membered Rings and Helicene Units, *Chem. Sci.*, **14(38)**, 10420-10428 (2023).

Mizuhata, Y.; Tokitoh, N., Germaaromatic Compounds, *Organogermanium Compounds: Theory, Experiment, and Applications*, 477-506 (2023).

Lv, X.; Gao, H.; Wu, F.; Liu, N.; Ueno, S.; Yang, X.; Zhang, T.; Aratani, N.; Yamada, H.; Qiu, F.; Shen, Z.; Xue, S., Highly Robust and Antiaromatic Rhenium(I) Rosarin, *Inorg. Chem.*, **62(12)**, 4747-4751 (2023).

Kitao, T.; Miura, T.; Nakayama, R.; Tsutsui, Y.; Chan, Y. S.; Hayashi, H.; Yamada, H.; Seki, S.; Hitosugi, T.; Uemura, T., Synthesis of Polyacene by Using a Metal-Organic Framework, *Nat. Synth.*, **2**, 848-854 (2023).

Chiga, Y.; Takahata, R.; Suzuki, W.; Mizuhata, Y.; Tokitoh, N.; Teranishi, T., Isomer-Selective Conversion of Au Clusters by Au(I) Thiolate Insertion, *Inorg. Chem.*, **62(26)**, 10049-10053 (2023). Iwai, K.; Mizuhata, Y.; Nakamura, T.; Goto, M.; Wakamiya, A.; Shimakawa, Y.; Tokitoh, N., Solid-State Chromism of Zwitterionic Triarylmethylium Salts, *Eur. J. Inorg. Chem.*, **26(31)**, e202300337 (2023).

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Mizuhata, Y.; Ijichi, W.; Nishino, R.; Kato, T.; Kayahara, E.; Yamago, S.; Tokitoh, N., Synthesis and Characterization of Novel Hydrodigermenide and Digermyne Radical Anion, *Polyhedron*, **244**, 116614 (2023).

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Yamada, H.; Matsuo, K., (*Invited*) 5,15-Diazatetrabenzoporphyrins: Evaluation as Organic Semiconductors, *ECS Meet. Abstr.*, **MA2023-01**, 1358, (2023).

Miyazaki, K.; Matsuo, K.; Hayashi, H.; Yamauchi, M.; Aratani, N.; Yamada, H., An Unsymmetrical 5,15-Disubstituted Tetrabenzoporphyrin: Effect of Molecular Symmetry on the Packing Structure and Charge Transporting Property, *Org. Lett.*, **25(40)**, 7354-7358 (2023).

Yamauchi, M.; Nakatsukasa, K.; Kubo, N.; Yamada, H.; Masuo, S., One-Dimensionally Arranged Quantum-Dot Superstructures Guided by a Supramolecular Polymer Template, *Angew. Chem. Int. Ed.*, **63(1)**, e202314329 (2023).

Wakioka, M.; Hatakeyama, K.; Sakai, S.; Seki, T.; Tada, K. I.; Mizuhata, Y.; Nakazato, T.; Koguchi, S.; Shibuya, Y.; Maruyama, Y.; Ayabe, M., Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation of Heteroarenes with Aryl Chlorides: Controlling Reactivity of Catalytic Intermediates via Dynamic Ligand Exchange, *Organometallics*, **42(24)**, 3454-3465 (2023).

Fujimori, S.; Mizuhata, Y.; Tokitoh, N., Recent Progress in the Chemistry of Heavy Aromatics, *Proc. Jpn. Acad., Ser. B.*, **99(10)**, 480-512 (2023).

Tsuji, S.; Tokitoh, N.; Yamada, H.; Mizuhata, Y., The Reduction of Metallabenzenes: Different Scenarios Highly Dependent on the Central Group 14 Elements, Si vs. Ge, *Chem. Asian J.*, **19(2)**, e202300945 (2023).

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Yamauchi, M.; Masuo, S., How to Arrange Quantum Dots?, *Monthly Chemistry*, **78(2)**, 70-71 (2023).

- Structural Organic Chemistry -

Hashikawa, Y.; Sadai, S.; Murata, Y., Bilateral π -Extension of an Open-[60]Fullerene in a Helical Manner, *Chem. Commun.*, **59**, 6560-6563 (2023).

Hashikawa, Y.; Murata, Y., C2-Insertion into a Fullerene Orifice, *Chem. Commun.*, **59(12)**, 1645-1648 (2023).

Sadai, S.; Hashikawa, Y.; Murata, Y., Open-[60]Fullerene-Aniline Conjugates with Near-Infrared Absorption, *RSC Adv.*, **13(21)**, 14575-14579 (2023).

Hashikawa, Y.; Sadai, S.; Murata, Y., Synthesis of Open-[70] Fullerenes Bearing Huge Orifices, *Chem. Commun.*, **59**, 7387-7390 (2023).

Briš, A.; Murata, Y.; Hashikawa, Y.; Margetić, D., Utilization of *Sym*-Tetrazines as Guanidine Delivery Cycloaddition Reagents, *J. Mol. Struct.*, **1272**, 134207 (2023).

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HAKUBI PROJECT

— Optoelectronic Energy Recycling and Quantum Cooperative Effects in Semiconductor Nanostructures —

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INTERNATIONAL RESEARCH COLLABORATIONS

[Australia]

Monash University, Monash Biomedicine Discovery Institute

[Austria] Vienna University of Technology, Photonics Institute

[China, P.R.]

Chinese Academiy of Science, Changchun Institute of Applied Chemistry

Fudan University, School of Computer Science

Fudan University, School of Pharmacy

Peking University, Peking-Tsinghua Center for Life Sciences, College of Life Sciences

ShanghaiTech University, School of Information Science and Technology

South China University of Technology, School of Computer Science and Engineering

The University of Hong Kong, Department of Mathematics

Tsinghua University, Department of Chemistry

[Croatia] Ruđer Bošković Institute, Division of Organic Chemistry and Biochemistry

[Czech Republic] The Czech Academy of Sciences, Institute of Hydrobiology

[Finland] Aalto University, Department of Computer Science

[France] Centre National de la Recherche Scientifique

French Alternative Energies and Atomic Energy Commission (CEA), Laboratoire de Physiologie Cellulaire & Végétale

[Germany]

European Molecular Biology Laboratory

Heinrich-Heine-Universität Düsseldorf, Institut für Theoretische Chemie und Computerchemie

Karlsruhe Institute of Technology, Institute of Organic Chemistry

Technische Universität Dresden, Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP)

[India]

Birbal Sahni Institute of Palaeosciences

CSIR-National Institute for Interdisciplinary Sciences and Technology, Chemical Science and Technology Division

Indian Institute of Technology, Bombay, Department of Metallurgical Engineering & Materials Science Including Corrosion Science & Engineering

[Israel]

Ben-Gurion University of the Negev, Department of Computer Science

[Italy]

University of Naples "Federico II", Department of Chemical Sciences

[Norway] University of Bergen, Department of Biology

[Romania]

Extreme Light Infrastructure-Nuclear Physics (ELI-NP), Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH)

National Institute for Laser, Plasma and Radiation Physics

[Sri Lanka]

University of Colombo, Departmentof Chemistry

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National Yang Ming Chiao Tung University, Institute of Bioinformatics and Systems Biology

[Thailand]

Chiang Mai University, Center of Excellence in Materials Science and Technology

Chiang Mai University, Faculty of Science

Maejo University, School of Renewable Energy

Mahidol University, Faculty of Science

Naresuan University, Faculty of Science

Thailand Center of Excellence in Physics, Ministry of Higher Education, Science, Research and Innovation

Thailand National Metal and Materials Technology Center, Powder Metallurgy Research and Development Unit [the U.K.] Durham University, OEM Research Group, Department of Physics

University of St. Andrews, EaStCHEM School of Chemistry

University of St Andrews, Organic Semiconductor Centre, EaStCHEM School of Chemistry

[the U.S.]

Stony Brook University, Department of Materials Science and Chemical Engineering

The Ohio State University, Department of Microbiology & Department of Civil, Environmental, and Geodetic Engineering

University of South Florida, College of Marine Science

University of Michigan, Department of Chemical Engineering

University of California San Diego, Scripps Institution of Oceanography

SELECTED GRANTS

DIVISION OF SYNTHETIC CHEMISTRY — Organoelement Chemistry —

TOKITOH, Norihiro New Main Group Element Chemistry and Materials Science Based on Heavy Aryl Anions Grant-in-Aid for Scientific Research (S) 26 June 2019–31 March 2024

YAMADA, Hiroko Development Organic Donor-Acceptor Materials for the Cotrol of Dynamic Exciton Grant-in-Aid for Transformative Research Areas (A) 19 November 2020–31 March 2025

YAMADA, Hiroko Development of Pi-Expanded Aromatic Compounds Based on Precursor Approach Grant-in-Aid for Scientific Research (A) 1 April 2020–31 March 2023

MATSUO, Kyohei Development of n-Type Organic Semiconductors Using Main Group Element Complexes of Tetrabenzoporphyrins Grant-in-Aid for Scientific Research (C) 1 April 2022–31 March 2025

YAMAUCHI, Mitsuaki Control of Helical Arrangement of Quantum Dots Using Supramolecular Templates and the Realization of Circular Polarized Emission Grant-in-Aid for Early-Career Scientists 1 April 2022–31 March 2025

YUKIMOTO, Mariko Creation of Tautomerizable Heavy Amides Compounds Grant-in-Aid for Early-Career Scientists 1 April 2022–31 March 2024

- Structural Organic Chemistry -

MURATA, Yasujiro Developments of Nanoscale Laboratory by Sophisticated Chemical Transformation of Fullerenes Grant-in-Aid for Scientific Research (B) 1 April 2023–31 March 2026 MURATA, Yasujiro Synthesis and Photophysical Properties of Novel Chiral Nanocarbons Grant-in-Aid for Challenging Research (Exploratory) 30 June 2023–31 March 2025

HIROSE, Takashi Investigation on Chiral Molecular Wire Properties Based on pi-Extended Helical Molecules Grant-in-Aid for Scientific Research (B) 1 April 2023–31 March 2026

HIROSE, Takashi Creation of Chiral Molecular Functions Based on Precise Arrangement of Helical pi-Conjugated Molecules PRESTO, (Precursory Research for Embryonic Science and Technology), JST 1 December 2020–31 March 2024

HASHIKAWA, Yoshifumi Creation of Experimental Hydration Models Based on Spherical pi-Systems Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area) 1 April 2022–31 March 2024

- Synthetic Organic Chemistry -

OHMIYA, Hirohisa Flexible Conversion of Complex and Bulky Molecules Using Light Energy Grant-in-Aid for Transformative Research Areas (A) 1 April 2023–31 March 2028

OHMIYA, Hirohisa Radical-Enabled Organocatalytic Chemistry Grant-in-Aid for Scientific Research (A) 5 April 2021- 31 March 2025

NAGAO, Kazunori Catalytic Generation of Sulfur Cation Radical Species by Dynamic Exciton and its Application to Bond Formation Reactions Grant-in-Aid for Transformative Research Areas (A) 10 September 2021–31 March 2023

NAGAO, Kazunori Catalytic Generation of Carbocation without Acids and the Application to Bond Formation Reactions Grant-in-Aid for Early-Career Scientists 1 April 2021–31 March 2024

Abbreviations and Acronyms

AMED : Japan Agency for Medical Reserach and Development JSPS : Japan Society for the Promotion of Science JST : Japan Science and Technology Agency MEXT : Ministry of Education, Culture, Sports, Science and Technology NEDO : New Energy and Industrial Technology Development Organization METI : Ministry of Economy, Trade and Industry

- Advanced Inorganic Synthesis -

TERANISHI, Toshiharu Nanoscale Element Replacement Science: Structural Transformation of Nanocrystalline Phases and Development of Novel Functions Grant-in-Aid for Scientific Research (S) 26 June 2010, 21 March 2004

26 June 2019–31 March 2024

TERANISHI, Toshiharu Synthesis of Unprecedented Ordered Alloy Nanoparticles and Development of Their Structure-Specific Properties Grant-in-Aid for Challenging Research (Exploratory) 28 June 2019–31 March 2023

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TERANISHI, Toshiharu Fabrication of Unprecedented Alloy Cathode Catalysts Development of Technologies for Realizing a Hydrogen Society, NEDO 31 July 2020–31 March 2025

TAKAHATA, Ryo Modeling of Defects and Exploration of Novel Materials by Using Cadmium Chalcogenide Clusters with Definite Structures Grant-in-Aid for Early-Career Scientists 1 April 2021–31 March 2024

TAKAHATA, Ryo Development of Precise Control Methods for Nanomaterials with Multi-Functions Uncharted Territory Challenge 2050, NEDO 1 November 2021–30 September 2026

TAKEKUMA, Haruka Controlling Plasmonic Properties of Novel Ordered Alloy Nanoparticles Grant-in-Aid for Early-Career Scientists 1 April 2023–31 March 2026

TAKEKUMA, Haruka Creation of Platinum-Based Bimetallic Nanoparticles IRCCS Young Scientists Co-Creation Proposal Research Fund 1 April 2022–31 March 2023

SARUYAMA, Masaki Chemical Synthesis and Exploration of Concerted Optical Properties of Anisotropic Three-Dimensional Quantum Dot Superlattices Grant-in-Aid for Scientific Research (B) 1 April 2023–31 March 2027

SARUYAMA, Masaki Synthesis and Function of Diverse Three-Dimensional Inorganic Nanoparticle Superstructures Grant-in-Aid for Challenging Research (Exploratory) 30 July 2020–31 March 2023

SARUYAMA, Masaki Creation of Strucutre Specific Reaction Fields through Self-Assembly of Nanocrystals FOREST (Fusion Oriented Research for Disruptive Science and Technology), JST 1 April 2022–31 March 2025 SATO, Ryota Principle Study of Plasmonic Ordered Nanoalloys Grant-in-Aid for Scientific Research (B) 1 April 2023–31 March 2027

MATSUMOTO, Kenshi Inter-Element Miscibility Driven Rearrangement from Disordered to Long-Range Ordered Alloy Structures Grant-in-Aid for Early-Career Scientists 1 April 2022–31 March 2025

DIVISION OF MATERIALS CHEMISTRY — Chemistry of Polymer Materials —

TSUJII, Yoshinobu

Development of Next-Generation Monolithic Membrane Columns to Reduce Biopharmaceutical Purification Costs Go-Tech Project, The Small and Medium Enterprise Agency, METI 1 August 2023–1 May 2025

TSUJII, Yoshinobu Development of High-Performance Sliding Parts by Imparting

Concentrated Polymer Brushes (CPB) and Their Application to Equipment A-STEP (Adaptable and Seamless Technology Transfer Program through Target-driven R&D), JST

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TSUJII, Yoshinobu

Hierarchical Understanding and Control of Wear Phenomena on Ultra-Low Friction Polymer Brushes CREST (Core Research for Evolutional Science and Technology), JST 1 October 2021–31 March 2027

TSUJII, Yoshinobu

Development of Next-Generation Ship-Bottom Coating Films and Coating Processes for Energy Saving and Reduced Environmental Impact Environment Research and Technology Development Fund, ENCA (Environmental Partmetic and Concernition Access)

ERCA (Environmental Restoration and Conservation Agency) 1 April 2022–31 March 2024

KINOSE, Yuji

Synthesis of Asymmetric Polymer-Brush-Modified Nanorods and Formation of Their Ordered Structures Grant-in-Aid for Early-Career Scientists 1 April 2023–31 March 2026

ISHIDA, Koichiro

Construction of Polysaccharide-Nanofiber Monolayers by Interfacial Architectonics and Creation of Novel Scaffold Functions Grant-in-Aid for JSPS Research Fellow 8 April 2022–31 March 2024

- Polymer Controlled Synthesis -

YAMAGO, Shigeru

Development of New Fabrication Methods of Polymer Materials Based on the Structurally Controlled Hyperbranched Polymers Grant-in-Aid for Scientific Research (S) 5 July 2021–31 March 2026 YAMAGO, Shigeru International Research Center for Basic Organic Device Chemistry by True Integration of Synthesis and Device Core-to-Core Program, JSPS 1 April 2022–31 March 2026

TOSAKA, Masatoshi Aggregation Structure of Hyper-branched Block Copolymers in Solution Grant-in-Aid for Scientific Research (C) 1 April 2021–31 March 2024

KAYAHARA, Eiichi Creation of New Cyclic π -Conjugated Molecules for Realization of High Density Conjugation Grant-in-Aid for Transformative Research Areas (A) 10 September 2021–31 March 2023

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- Inorganic Photonics Materials -

MIZUOCHI, Norikazu Research of Quantum Sensing by Advanced Control of the Quantum State of NV Center in Diamond Grant-in-Aid for Scientific Research (A) 5 April 2021–31 March 2024

MIZUOCHI, Norikazu Development of Innovative Sensor Systems by Highly Sophisticated Control of Solid Quantum Sensors Q-LEAP (Quantum Leap Flagship Program), MEXT 1 November 2018–31 March 2028

MIZUOCHI, Norikazu Innovations Medicine and Life Sciences through the Application of Quantum Technology Q-LEAP (Quantum Leap Flagship Program), MEXT 1 April 2020–31 March 2030

MIZUOCHI, Norikazu Highly Sensitive Quantum Sensing Microscope Development Research for Elucidating Biological Phenomena CREST (Core Research for Evolutional Science and Technology), JST 1 October 2023–31 March 2029

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MORIOKA, Naoya Study of Spin-Optical-Charge Dynamics of Defects in Silicon Carbide for Highly Efficient Electrical Spin Readout Grant-in-Aid for Scientific Research (B) 1 April 2022–31 March 2025 MORIOKA, Naoya Exploring Control of Localized Spins Based on Electrical Spin Injection in Silicon Carbide Grant-in-Aid for Research Activity Start-up 30 August 2021–31 March 2023

HERBSCHLEB, Ernst David Enhanced Quantum Sensing with a Nitrogen-Vacancy Centre as Gateway to the Electron Spin of Phosphorus Grant-in-Aid for Early-Career Scientists 1 April 2022–31 March 2024

NISHIKAWA, Tetsuri Investigation of Carrier Transport Mechanism for Photocurrent-Detected Magnetic Resonance on Color-Center Spins in Silicon Carbide Grant-in-Aid for Research Activity Start-up 31 August 2023–31 March 2025

- Nanospintronics -

ONO, Teruo Ferrimagnetic Spintronics and Device Application Grant-in-Aid for Scientific Research (S) 31 August 2020–31 March 2025

ONO, Teruo he Unraveling the Mechanism of Superconductive Diode Effect and Creating Non-Volatile Superconductive Diode Grant-in-Aid for Challenging Research (Pioneering)

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SHIOTA, Yoichi

Polarization Control of Spin Wave Spin Current and Its Device Application Grant-in-Aid for Scientific Research (B) 1 April 2022–31 March 2025

HISATOMI, Ryusuke

Creation of Highly Efficient Optical Photon-Microwave Conversion Using Disk-Shaped Ferromagnetic Thin Films Grant-in-Aid for Early-Career Scientists 1 April 2022–31 March 2024

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Opto-Spin-Mechanics Using Surface Acoustic Waves PRESTO (Precursory Research for Embryonic Science and Technology), JST 1 November 2020–31 March 2024

KARUBE, Shutaro Development of Novel Spin Current Control Technology Based on Exchange Interaction Grant-in-Aid for Early-Career Scientists 1 April 2022–31 March 2025

KARUBE, Shutaro Creation of Innovative Information Carrier Devices by Multifunctional Spin Oxides PRESTO (Precursory Research for Embryonic Science and Technology), JST 1 October 2022–31 March 2025 NARITA, Hideki Control of Superconductivity by Noncollinear Magnetism Grant-in-Aid for Early-Career Scientists 1 April 2021–31 March 2024

NARITA, Hideki Creation of Innovative Quantum Control Technology Using Hybrid Superconductors PRESTO (Precursory Research for Embryonic Science and Technology), JST 1 October 2023–31 March 2025

DIVISION OF BIOCHEMISTRY

- Biofunctional Design-Chemistry -

FUTAKI, Shiroh Intracellular Fate of Extracellular Fine Particles and the Control System CREST (Core Research for Evolutionary Science and Technology), JST 1 October 2018–1 March 2024

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- Molecular Biology -

AOYAMA, Takashi Roles of Phosphoinositid Signaling in Plant Cell Morphogenesis Grant-in-Aid for Scientific Research (B) 1 April 2021–31 March 2024

TSUGE, Tomohiko Molecular Mechanism Governing Plant Plasticity through PremRNA 3'UTR Regulation Grant-in-Aid for Scientific Research (C) 1 April 2022–31 March 2025 KATO, Mariko Study on the Involvement of Phosphoinositides in Pollen Germination Grant-in-Aid for Scientific Research (C) 1 April 2021–31 March 2025

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UESUGI, Motonari Development of Artificial Chaperones Grant-in-Aid for Transformative Research Areas (A) 16 June 2022–31 March 2024

UESUGI, Motonari Chemical Biology of Cellular Self-Assemblies Grant-in-Aid for Scientific Research (A) 1 April 2022–31 March 2025

UESUGI, Motonari Designer Melanin for Analyzing and Controlling Cells Grant-in-Aid for Challenging Research (Exploratory) 9 July 2021–31 March 2023

UESUGI, Motonari Intracellular Analysis of LLPS Status Grant-in-Aid for Challenging Research (Exploratory) 30 June 2023–31 March 2025

UESUGI, Motonari Asian Chemical Biology Intiative Core-to-Core Program, JSPS 1 April 2022–31 March 2025

UESUGI, Motonari PD-1 Blockade Caner Immunotherapy Combined with Small Molecule Activators of T Cell Fatty Acid Oxidation P-PROMOTE (Project for Promotion of Cancer Research and Therapeutic Evolution), AMED 20 May 2022–31 March 2024

UESUGI, Motonari Grand Design Platform and Database for the Development of Innovative Adjuvant and Vaccine Carrier Program on R&D of New Generation Vaccine Including New Modality Application, AMED 1 July 2022–31 March 2027

SATO, Shinichi Understanding Cellular Function with Short RNAs and Small Molecules Grant-in-Aid for Scientific Research (B) 1 April 2020–31 March 2023

SATO, Shinichi New Technologies for RNA Structural Regulation that Enables the Control and Analysis of Cellular Function Grant-in-Aid for Scientific Research (B) 1 April 2023–31 March 2026

SATO, Shinich A New Oligonucleotide Therapeutics that Induces a Cooperative RNA G-Quadruplex Formation for Gene Silencing Grant-in-Aid for Challenging Research (Pioneering) 9 July 2021–31 March 2025 PERRON, Amelie Live and Let Die: Orchestrating Aggregation of Eye Pigments with Organic Molecules Grant-in-Aid for Scientific Research (C) 1 April 2023-31 March 2026

ABO, Masahiro Development of Self-Assembling Chemicals which Have Chaperone Activity in Live Cells Grant-in-Aid for Scientific Research (C) 1 April 2021-31 March 2024

TAKEMOTO, Yasushi Exploration of Radical-Sensitive Signal Peptide Grant-in-Aid for Scientific Research (C) 1 April 2022-31 March 2025

TAKEMOTO, Yasushi Understanding and Application of Radical-Sensitive Peptide Takeda Science Foundation 1 September 2021-31 May 2024

TAKEMOTO, Misao Mechanistic Analysis for the Immune Activation of T Cells by Covalent Natural Compounds Grant-in-Aid for Scientific Research (C) 1 April 2022-31 March 2025

DIVISION OF ENVIROMENTAL CHEMISTRY Molecular Materials Chemistry —

KAJI, Hironori Material Design Based on Dynamic Excition and their Applications Grant-in-Aid for Transformative Research Areas (A) 19 November 2020-31 March 2025

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SUZUKI, Katsuaki

Spatiotemporal Analysis of Dynamic Exciton by Solid-State NMR Grant-in-Aid for Transformative Research Areas (A) 19 November 2020-31 March 2025

TANAKA, Hiroyuki Development of Multiple-Resonance Thermally Activated Delayed Fluorescent Molecules with Excellent Circularly Polarized Luminescence Property Grant-in-Aid for Challenging Research (Exploratory) 1 July 2023-31 March 2025

- Hydrospheric Environment Analytical Chemistry -

SOHRIN, Yoshiki Ocean Section Diagnosis on the Basis of Stoichiometry and Stable Isotope Ratios of Trace Metals Grant-in-Aid for Scientific Research (A) 1 April 2019-31 March 2023

TAKANO, Shotaro Isotopic Analysis for Estimating the Sources of Particulate Trace Metals in the Ocean Grant-in-Aid for Early-Career Scientists 1 April 2020-31 March 2023

ZHENG, Linjie Speciation and Sectional Distribution of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in the South Pacific and Indian Oceans Grant-in-Aid for Early-Career Scientists 1 April 2021-31 March 2024

- Chemistry for Functionalized Surfaces -

HASEGAWA, Takeshi Evolution of Near-Infrared Spectroscopy for Materials Structure Analysis: Development of NIR-MAIRS Grant-in-Aid for Scientific Research (B) 1 April 2022-31 March 2026

HASEGAWA, Takeshi Innovation in Control of Physical Properties of Polymer Thin-Film Materials by Micro-Morphology Analysis of Amorphous Grant-in-Aid for Challenging Research (Exploratory) 9 July 2021-31 March 2024

MORI, Taizo

Dynamic Response of Molecular Machines at the Air-Water Interface Using Second Harmonic Generation Grant-in-Aid for Scientific Research (C) 1 April 2023-31 March 2028

SHIOYA, Nobutaka

Visualization of Monolayer Structures Specifically Formed by Functional Organic Materials at the Substrate Interface Grant-in-Aid for Early-Career Scientists 1 April 2022-31 March 2025

— Molecular Microbial Science —

KURIHARA, Tatsuo Molecular Basis for Generation of the Diversity of Bacterial Membrane Phospholipid Acyl Chains and Mechanisms Underlying Their Physiological Functions Grant-in-Aid for Scientific Research (B) 1 April 2021-31 March 2024

KURIHARA, Tatsuo

Dissection of the Molecular Basis of Membrane Vesicle Biogenesis and Construction of an Extracellular Platform for Substance Production by Using a Hyper-Vesiculating Bacterium Grant-in-Aid for Challenging Research (Pioneering) 30 July 2020-31 March 2023

KURIHARA, Tatsuo

Enzymatic Manipulation of Biomembrane Lipids to Enhance Cellular Function Grant-in-Aid for Challenging Research (Exploratory) 30 June 2023-31 March 2025

KAWAMOTO, Jun

Elucidation of Molecular Mechanism of Extracellular Membrane Vesicle Production by Bacteria and Its Application Grant-in-Aid for Scientific Research (B) 1 April 2023-31 March 2026

KAWAMOTO, Jun

A Novel Platform for Functional Nanoparticle -the Synthesis Mechanism of Unique Outer-Membrane Vesicles of Bacteria and Its Application-Grant-in-Aid for Scientific Research (C)

1 April 2020-31 March 2023

KAWAMOTO, Jun Exploration and Application of Outer Membrane Vesicle-Producing Bacteria as a Foundation for New Nano-Material Development Fund for the Promotion of Joint International Research (International Collaborative Research) 8 September 2023–31 March 2027

OGAWA, Takuya Study on the Metabolic Conversion of Omega-3 Polyunsaturated Fatty Acids through a Reconsideration of Beta-Oxidation Pathway Grant-in-Aid for Scientific Research (C) 1 April 2021–31 March 2024

DIVISION OF MULTIDISCIPLINARY CHEMISTRY — Polymer Materials Science —

TAKENAKA, Mikihito 4D Analysis of Grazing Incidence Scattering to Reveal Adhesion Processes at the Adhesive Interface Mirai Program, JST 1 November 2018–31 March 2028

OGAWA, Hiroki Non-Equilibrium MI Scheme Shortens Future Material Development Feasibility Study Program, NEDO 10 May 2023–31 March 2025

OGAWA, Hiroki Development of a Recycled Plastics Databank to Improve the Circurability SIP, ERCA (Environmental Restoration and Conservation Agency) 1 October 2023–31 March 2028

- Molecular Rheology -

MATSUMIYA, Yumi Molecular Dynamics of Associative Polymers and Its Experimental Validation: Effect of Dissociation Equilibrium on Entanglement Relaxation Modes Grant-in-Aid for Scientific Research (B) 1 April 2021–31 March 2024

SATO, Takeshi Development of Coarse-Grained Molecular Model for Predicting Dynamics of Entangled Associating Polymers Grant-in-Aid for Early-Career Scientists 1 April 2021–31 March 2024

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- Molecular Aggregates -

WAKAMIYA, Atsushi Fundamental Chemical Research for Efficient Lead Free Perovskite Solar Cells Grant-in-Aid for Scientific Research (A) 5 April 2021–31 March 2024 WAKAMIYA, Atsushi Pb-Free Perovskite Solar Cells Consisting of Sn Mirai Full-scale R&D Project, JST 1 April 2022–31 March 2027

WAKAMIYA, Atsushi Development of Practical Technology for Perovskite Solar Module with High Installation Flexibility Green Innovation Fund Projects ,NEDO 27 December 2021–31 March 2026

WAKAMIYA, Atsushi Development of Film-Type Perovskite Solar Module with High Degree of Freedom Design Development of Technologies to Promote Photovoltaic Power Generation as a Primary Power Source, NEDO 13 July 2020–31 March 2025

MURDEY, Richard Ageing and Passivation Effects in Perovskite Solar Cells Grant-in-Aid for Scientific Research (C) 1 April 2019–31 March 2023

NAKAMURA, Tomoya Two-Dimensionally Expanded pi-Systems for High-Performance Tin Perovskite Solar Cells Grant-in-Aid for Early-Career Scientists 1 April 2021–31 March 2023

TRUONG, Minh Anh Development of Multipodal Hole-Transporting Monolayer Materials for High Performance Perovskite Solar Cells Grant-in-Aid for Early-Career Scientists 1 April 2022–31 March 2024

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE — Particle Beam Science —

WAKASUGI, Masanori Precise Measurement of Charge Density Distribution of Sn Unstable Isotopes by Advanced Innovative SCRIT Electron Scattering Grant-in-Aid for Scientific Research (S) 12 April 2023–31 March 2028

WAKASUGI, Masanori Development of Stationary Target for Unstable Nuclei for Application to Research of Nuclear Reaction Grant-in-Aid for Challenging Research (Pioneering) 30 July 2020–31 March 2023

WAKASUGI, Masanori Development of RFQ-Type Isobar Filters Leading Inovative Research on Unstable Nuclear Reactions Grant-in-Aid for Challenging Research (Pioneering) 30 June 2023–31 March 2026

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OGAWARA, Ryo Development of Internal Active Target for Beam Recycle Techniques Grant-in-Aid for Early-Career Scientists 1 April 2022–31 March 2024 OGAWARA, Ryo Development of Beam Recycle Techniques for Advanced Research on Nuclear Reactions with Rare RI FOREST (Fusion Oriented Research for Disruptive Science and Technology), JST 1 April 2023–31 March 2030

TONGU, Hiromu Mapping System Using High-Speed Scanning in Cryogenic Environment for Superconductor State Inspection Grant-in-Aid for Scientific Research (C) 1 April 2022–31 March 2025

- Laser Matter Interaction Science -

TOKITA, Shigeki Development of Mid-Infrared High-Power Ultrashort Pulse Lasers and Its Application to Soft-Matter Micro-Processing Grant-in-Aid for Scientific Research (B) 1 April 2021-31 March 2024

TOKITA, Shigeki The Power Laser DX Platform Project for Promoting Public Utilization of Advanced Research, MEXT 1 April 2021-31 March 2026

TOKITA, Shigeki Formation of Ultrashort Femtosecond Pulses in the Mid-Infrared Range Based on Iron-Doped Chalcogenides for Problems of Nonlinear Optics of Media with a Reduced Dimension Bilateral Joint Research Projects, JSPS 1 April 2021-31 March 2023

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TOKITA, Shigeki Pioneering of a High-Intensity Coherent X-Ray Generation Method Using an Ultrahigh-Intensity Mid-Infrared Laser Matsuo Academic Research Grant, MATSUO Foundation 1 December 2023–31 March 2025

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TOKITA, Shigeki Development of High-Intensity Mid-Infrared Lasers for Realizing Compact Coherent X-Ray Sources Research Grant, Research Foundation for Opto-Science and Technology 1 January 2023–31 December 2024

TOKITA, Shigeki Micromachining of Transparent Resin Using Mid-Infrared Pulsed Lasers AMADA Research and Development Grant, The AMADA Foundation

26 September 2020-31 March 2024

TOKITA, Shigeki

Development of High-Intensity Coherent X-Ray Generation Method Supporting Program for Unique Exploratory Investigation Team Studies (SPIRIT2), Kyoto University 1 April 2023-31 March 2025

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OKAZAKI, Daiki Research on a Novel Burst Pulse Generation Technique for Efficient Femtosecond Laser Processing Encouragement Research Grant, The Amada Foundation 1 October 2023–31 March 2026

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KANAI, Tsuneto

Development of a Mid-IR Laser-Driven X-Ray Source for Zeptosecond Particle Physics Matsuo Academic Research Grant, MATSUO Foundation 1 December 2022-31 March 2024

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HASHIDA, Masaki Operando Measurements Using Advanced Beams to Study the Mechanism of Fine Structure Formation Basic Foundational Research: "Next-Generation Laser" Projects, Q-LEAP (Quantum Leap Flagship Program), MEXT

1 April 2020-31 March 2029

- Electron Microscopy and Crystal Chemistry -

HARUTA, Mitsutaka Visualization of Electron Orbital Using TEM Grant-in-Aid for Scientific Research (B) 1 April 2022-31 March 2025

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

- Synthetic Organotransformation -

NAKAMURA, Masaharu Iron-Catalyzed Cross Coupling: Quantum Control on Multi-Spin Pathways Grant-in-Aid for Scientific Research (B) 1 April 2023–31 March 2026

ISOZAKI, Katsuhiro Triple-Layer Core-Shell Metal Nanocluster Synthesis Driven by Interligand Hydrogen Bonds Grant-in-Aid for Challenging Research (Exploratory) 30 June 2023–31 March 2025

DOBA, Takahiro Iron-Catalyzed Carbon–Heteroatom Bond Formation Reactions through pi-Plane Activation Research Activity Start-up 31 August 2023–31 March 2025

DOBA, Takahiro Development of Iron-Catalyzed Carbon–Heteroatom Bond Formation Reactions Research grant from the Institute of Synthetic Organic Chemistry 1 October 2023–30 September 2024

NAKAGAWA, Yuka Pioneering Catalytic Reactions for Direct Synthesis of Functional Polymers from Wood Grant-in-Aid for Early-Career Scientists 1 April 2023–31 March 2026

NAKAGAWA, Yuka Development of Molecular Complex Catalysts for Converting Wood into Functional Materials PRESTO, (Precursory Research for Embryonic Science and Technology), JST 30 September 2023–30 March 2027

MINEO, Keito Integrated Scenario Analysis of Environmental Impacts and Economic Potential of Forest Management and Wood Uses Daigas Research Grants for Young Researchers, Kyoto University Open Innovation Institute

8 February 2023–7 February 2024

IMAI, Makiko Analysis of Lignin Decomposition Mechanism That Produce Nanosheet Cellulose Grant-in-Aid for Early-Career Scientists 1 April 2023–31 March 2026

- Advanced Solid State Chemistry -

SHIMAKAWA, Yuichi Construction of Physical Property Correlation Based on Entropy and Creation of New Thermal Control Materials Grant-in-Aid for Scientific Research (S) 12 April 2023–31 March 2028

SHIMAKAWA, Yuichi
Exploration of Functional Transition-Metal Oxides and Their
Structure-Property Relationships
AdCORP (Advanced International Collaborative Research
Program), JST
1 April 2023–31 March 2027

- Organometallic Chemistry -

OHKI, Yasuhiro Synthesis and Reactions of Bio-Inspired Molecular Metal-Hydride Compounds Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area) 1 April 2021–31 March 2023

OHKI, Yasuhiro Synthesis of Iron-Containing Cluster Complexes and Reducing Reactions with Multiple Metals Grant-in-Aid for Scientific Research (B) 1 April 2023–31 March 2026

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OHKI, Yasuhiro Electron Transfer Networks of Transition Metal Cluster Complexes for Catalytic Applications CREST (Core Research for Evolutional Science and Technology), JST 1 October 2021–31 March 2027

TANIFUJI, Kazuki CO₂/CO Reduction into Short-Chain Hydrocarbons Promoted by Cuboidal Metal-Sulfur Clusters Grant-in-Aid for Scientific Research (C) 1 April 2022–31 March 2025

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HIGAKI, Tatsuya Creation of Novel Cluster Nanomagnets with Strong Exchange Interactions Grant-in-Aid for Early-Career Scientists 1 April 2023–31 March 2025

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- Nanophotonics -

KANEMITSU, Yoshihiko Fusing Nanomaterials and Strong Electric Field Nonlinear Optics for New Advances in Photonics Grant-in-Aid for Specially Promoted Research 23 April 2019–31 March 2024

KANEMITSU, Yoshihiko Optical Responses of Ordered Alloy Nanomaterials and Nanomaterial-Based Superstructures CREST (Core Research for Evolutional Science and Technology), JST 1 October 2021–31 March 2027

HIRORI, Hideki Phononic Strong Coupling by THz Metamaterial and Its Applications to Material Control Grant-in-Aid for Scientific Research (B) 1 April 2021–31 March 2025

YUMOTO, Go

Development of Polarization-Resolved Pump-Probe Microscopy and Study of Rashba Spin-Optoelectronics in Atomically Thin Materials Grant-in-Aid for Early-Career Scientists 1 April 2023–31 March 2025

TAHARA, Hirokazu Spatial and Temporal Super-Resolution Method for Revealing Quantum Cooperative Processes in Semiconductor Nanostructures Grant-in-Aid for Scientific Research (B) 1 April 2022–31 March 2026

TAHARA, Hirokazu Development of Nanostructured Semiconductor-Photon Coupled Systems for Giant Optoelectronic Amplification Grant-in-Aid for Challenging Research (Exploratory) 30 June 2023–31 March 2025

TAHARA, Hirokazu Development of Efficient Optoelectronic Devices with Quantum Cooperativity in Nanomaterial Superstructures PRESTO (Precursory Research for Embryonic Science and Technology), JST 1 October 2023–31 March 2027

BIOINFORMATICS CENTER — Chemical Life Science —

OGATA, Hiroyuki Virus-Driven Clockwork in Lower Tropic Level Marine Ecosystem and Its Impact on the Ocean Grant-in-Aid for Scientific Research (S) 5 July 2021–31 March 2026

OGATA, Hiroyuki Aggregate-Biosphere: Unveiling Hidden Regulatory Processes in the Oceanic Carbon Cycle Grant-in-Aid for Scientific Research (S) 26 June 2019–31 March 2024

OGATA, Hiroyuki Ecology of Giant viruses Inhabiting the Aphotic Zone of the Sea Grant-in-Aid for Scientific Research (A) 1 April 2022–31 March 2026 OGATA, Hiroyuki Molecular Ecological Mechanism of Bloom Disintegration by Viral Infection Grant-in-Aid for Scientific Research (A) 1 April 2022–31 March 2027

OGATA, Hiroyuki Study of Giant Virus Ecology and Virus-Host Interaction in Aquatic Environments Grant-in-Aid for Scientific Research (B) 1 April 2020–31 March 2023

OGATA, Hiroyuki Virus-Host Database Grant-in-Aid for Publication of Scientific Research Results (Database) 1 April 2020–31 March 2025

ENDO, Hisashi Viral Infection and Its Control Mechanisms of Marine Plankton Communities as Revealed by Dissolved Ribosomal RNA Grant-in-Aid for Scientific Research (B) 1 April 2022–31 March 2026

ENDO, Hisashi Plankton Communities Contributing to Marine Biological Pump on the Global Scale Grant-in-Aid for Scientific Research (B) 1 April 2022–31 March 2025

ENDO, Hisashi Experimental Investigation of the Effects of Phytoplankton Diversity on Ecosystem Functioning in the Ocean Grant-in-Aid for Early-Career Scientists 1 April 2019–31 March 2023

ENDO, Hisashi A Novel Dynamics Analysis of Marine Plankton Based on Genetic Information in the Dissolved Fraction of Seawater CREST (Core Research for Evolutional Science and Technology), JST 1 October 2023–31 March 2029

ENDO, Hisashi

A Novel Dynamics Analysis of Marine Plankton Based on Genetic Information in the Dissolved Fraction of Seawater PRESTO (Precursory Research for Embryonic Science and Technology), JST 1 October 2023–31 March 2027

OKAZAKI, Yusuke Unveiling the Organic Matter Dynamics Functioning in Lake Hypolimnion Grant-in-Aid for Scientific Research (A) 1 April 2022–31 March 2026

OKAZAKI, Yusuke Elucidating the Molecular Heterogeneity of Dissolved Organic Matter That Governs Its Long-Term Persistence Grant-in-Aid for Scientific Research (B) 1 April 2022–31 March 2025

OKAZAKI, Yusuke Microbial Nitrogen Pump: Bacterial Semi-Labile Dissolved Organic Nitrogen as a Nutrient Transport Pathway in Aquatic Systems Grant-in-Aid for Scientific Research (B) 1 April 2021–31 March 2024 OKAZAKI, Yusuke Who is the Host of Uncultivated Viruses? Linking Viral and Bacterial Genomes in the Environment Grant-in-Aid for Early-Career Scientists 1 April 2022–31 March 2025

OKAZAKI, Yusuke Developing a High-Resolution Eco-Genomics Platform through Inter-Lake Comparisons FOREST (Fusion Oriented Research for Disruptive Science and Technology), JST 1 April 2023–31 March 2030

OKAZAKI, Yusuke Challenging Dry Questions in Environmental Microbiology and Virology from Wet Kyoto University 125th Anniversary Fund Kusunoki 125 13 September 2021–31 March 2025

HIKIDA, Hiroyuki Diversity of Giant Virus Infection Strategy Grant-in-Aid for Early-Career Scientists 1 April 2022–31 March 2025

HIKIDA, Hiroyuki Development of Novel Gene Engineering Technology Utilizing Giant Viruses Strategic Basic Research Programs ACT-X, JST 1 October 2022–31 March 2025

- Mathematical Bioinformatics -

AKUTSU, Tatsuya Advanced Studies and Developments on Discrete Preimage Problems Grant-in-Aid for Scientific Research (A) 1 April 2022–31 March 2027

AKUTSU, Tatsuya Analysis and Control of Steady States of Multiple Biological Networks Grant-in-Aid for Challenging Research (Exploratory) 30 June 2022–31 March 2025

TAMURA, Takeyuki Algorithms for Metabolic Network Design for Producing Useful Substances Grant-in-Aid for Scientific Research (B) 1 April 2020–31 March 2025

MORI, Tomoya Establishment of the Method for Biological Tissue Domain Estimation and Analysis Based on Spatial Omics Data Grant-in-Aid for Scientific Research (C) 1 April 2023–31 March 2026

- Bio-knowledge Engineering -

MAMITSUKA, Hiroshi Development of Next Generation Plastic Materials Based on Structurally Controlled Hyperbranched Polymers Grant-in-Aid for Scientific Research (S) 5 July 2021–31 March 2026 MAMITSUKA, Hiroshi Latent Data Structure Estimation through Integrating Diverse Data Grant-in-Aid for Scientific Research (B) 1 April 2022–31 March 2025

MAMITSUKA, Hiroshi Developing Machine Learning Based Bioinformatics to Decipher Hidden Biology of Depression Symptoms Grant-in-Aid for JSPS Fellows 13 November 2020–31 March 2023

NGUYEN, Hao Canh Machine Learning on Large Graphs Grant-in-Aid for Scientific Research (C) 1 April 2018–31 March 2023

NGUYEN, Hao Canh Machine Learning for Structure-Rich Data-Scarce Domains Grant-in-Aid for Scientific Research (C) 1 April 2022–31 March 2025

THESES

AKAGI, Chika D Sc, Kyoto University "Study on Ribosome-related Gene Expression during Light Germination of *Arabidopsis thaliana*" Supervisor: Prof AOYAMA, Takashi 23 March 2023

FUNADA, Shinsaku D Sc, Kyoto University "Magnetic Resonance Measurements in Ferrimagnets with Compensation Points" Supervisor: Prof ONO, Teruo 17 January 2023

HIRAI, Yusuke D Pharm Sci, Kyoto University "Cytosolic Protein Delivery Using Lipid Nanoparticles" Supervisor: Prof FUTAKI, Shiroh 24 March 2023

HU, Shuaifeng D Sc, Kyoto University "Surface Modifications of Mixed Tin-Lead Halide Perovskite Films for Solar Cells" Supervisor: Prof WAKAMIYA, Atsushi 23 March 2023

IMAMURA, Yuji D Eng, Kyoto University "Advanced Control of Polymer Structure Based on Multiple Control in Radical Polymerization" Supervisor: Prof YAMAGO, Shigeru 23 May 2023

JIANG, Yuhan D Eng, Kyoto University "Development of Practical Organotellurium-Mediated Radical Polymerization Based on Polymerization and Separation in a Two-phase System" Supervisor: Prof YAMAGO, Shigeru 23 May 2023

JIN, Shuyu D Med, Kyoto University "Self-Assembling Small-Molecule Adjuvants as Antigen Nano-Carriers" Supervisor: Prof UESUGI, Motonari 23 March 2023

KOSUGI, Yoshihisa D Sci, Kyoto University "Synthesis and Evaluation of Transition Metal Oxides Exhibiting Caloric Effects" Supervisor: Prof. SHIMAKAWA, Yuichi 23 March 2017

LI, Ruiming D Inf, Kyoto University "Analysis of Biological Networks by Graph Theory-Based Methods" Supervisor: Prof AKUTSU, Tatsuya 23 March 2023 MAEHARA, Yoshiki M Sc, Kyoto University "Beam Dynamics of RUNBA and Developments of Dorrection Devices, EDC and ADC" Supervisor: Prof WAKASUGI, Masanori 23 March 2023

NGUYEN, Anh Duc D Pharm Sc, Kyoto University "Establishing Advanced Deep Learning Models for Predicting Drug Side Effects" Supervisor: Prof MAMITSUKA, Hiroshi 23 March 2023

NISHIKAWA, Tetsuri D Eng, Kyoto University "Development of Electrical Detection Techniques of Color Centers" Spins in Diamond and Silicon Carbide" Supervisor: Prof MIZUOCHI, Norikazu 23 March 2023

NISHIO, Kosuke D Med, Kyoto University "Magnetic Control of Cells by Chemical Fabrication of Melanin" Supervisor: Prof UESUGI, Motonari 23 March 2023



THE 123RD ICR ANNUAL SYMPOSIUM

(1 December 2023)

ORAL PRESENTATION

OKAZAKI, Daiki (Laser Matter Interaction Science) "Development of Mid-Infrared Femtosecond Lasers and Their Applications"

YAMAUCHI, Mitsuaki (Organoelement Chemistry) "Construction of Highly Ordered Quantum Dots and Organic Molecules with a Supramolecular Approach"

KINOSE, Yuji (Chemistry of Polymer Materials) "Anchoring Property on Zero Azimuthal Anchoring Surface"

- ICR Award for Young Scientists -

TRUONG, Minh Anh (Molecular Aggregates) "Tripodal Triazatruxene Derivative as a Face-on Oriented Hole-Collecting Monolayer for Efficient and Stable Inverted Perovskite Solar Cells"

MENG, Lingjie (Chemical Life Science) "Mirusviruses Link Herpesviruses to Giant Viruses"

- ICR Award for Graduate Students -

CHO, Kenichi (Nanophotonics)

"Exciton-Phonon and Trion-Phonon Couplings Revealed by Photoluminescence Spectroscopy of Single CsPbBr₃ Perovskite Nanocrystals"

ZHANG, Zhenya (Nanophotonics) "Generation of Third-Harmonic Spin Oscillation from Strong Spin Precession Induced by Terahertz Magnetic near Fields"

TOH, Kohei (Chemical Biology) "Chemoproteomic Identification of Blue-Light-Damaged Proteins"

- ICR Grants for Promoting Integrated Research -

HISATOMI, Ryusuke (Nanospintronics) "Study of Phonon Angular Momentum Using Impulsive Stimulated Raman Scattering"

ABO, Masahiro (Chemical Biology) "Development of Chemical Tools for Magnetic Manipulation of Biomolecules"

TAKAHATA, Ryo (Advanced Inorganic Synthesis); ISOZAKI, Katsuhiro (Synthetic Organotransformation) "Development of a Connection-Number-Controlling Method for

Nanoparticles"

HIKIDA, Hiroyuki (Chemical Life Science) "Transcriptome Analysis in Virus-Infected Non-Model Organisms"

TRUONG, Minh Anh (Molecular Aggregates) "Elucidating the Structure of Hole Collecting Monolayer in Perovskite Solar Cell"

POSTER PRESENTATIONS

- LW : Laboratory Whole Presentation
- LT : Laboratory Topic
- GE : General Presentation

- Organoelement Chemistry -

LW "Research Topics of Organoelement Chemistry Laboratory"

GE NISHINO, Ryohei; TOKITOH, Norihiro; YAMADA, Hiroko;
 MIZUHATA, Yoshiyuki
 "Development of a Single Germanium Atom Transfer Reagent"

- Structural Organic Chemistry -

LW "Recent Research Activities in Structural Organic Chemistry"

 $\underline{\text{GE}}$ HU, Weizhe; MURATA, Yasujiro; HIROSE, Takashi "Non-Linear Molecular Spring Properties of a Dibenzo[c,u][7] helicene Derivative Derived from Intramolecular Non-Covalent Interactions"

- Synthetic Organic Chemistry -

GE NAKAGAWA, Masanari; NAGAO, Kazunori; OHMIYA, Hirohisa

"A Light-Driven Hybrid Catalysis Enabling Construction of Azetidine via C-H Bond Activation"

- Advanced Inorganic Synthesis -

LW "Research Topics of Advanced Inorganic Synthesis"

GE ZHU, Lingkai; SARUYAMA, Masaki; TERANISHI, Toshiharu "Synthesis of 3D Ag Nanoparticle Superlattices and Their Structure-Specific Functions"

- Chemistry of Polymer Materials -

w "Recent Researches in Chemistry of Polymer Materials Laboratory"

GE SEIKE, Yuki; KINOSE, Yuji; TSUJII, Yoshinobu

"Synthesis of Concentrated Polymer Brushes with Larger Thickness via Improved Livingness in Surface-Initiated Controlled Radical Polymerization"

— Polymer Controlled Synthesis —

GE TONG, Tianxiang; KIBUNE, Masato; TOSAKA, Masatoshi; MATSUMIYA, Yumi; WATANABE, Hiroshi; YAMAGO, Shigeru "Synthesis of Structurally Controlled Dendritic Hyperbranched Polyacrylates by TERP and Their Rheological Properties"

GE MARU, Kosuke; ZHENG, Leshang; KAYAHARA, Eiichi; YAMAGO, Shigeru

"Synthesis of Cyclic π -conjugated Oligomers by the Insertion of Alkynes and Isocyanides into Cycloparaphenylene Metal Complexes"

— Inorganic Photonics Materials —

LW "Research Introduction of Inorganic Photonics Materials"

- Nanospintronics -

GE KAWARAZAKI, Ryo

"Spin Injection into a Superconductor without Inversion Symmetry"

GE TAGA, Kotaro; KOMIYAMA, Haruka; MATSUMOTO, Hiroki; HISATOMI, Ryusuke; NARITA, Hideki; KARUBE, Shutaro; MORIYAMA, Takahiro; SHIOTA, Yoichi; ONO, Teruo "Frequency and Magnetic Field Angle Dependences of the Coupling between Spin Wave and Surface Acoustic Wave in NiFe Thin Film"

- Biofunctional Design-Chemistry -

W "Recent Research in the Laboratory of Biofunctional Design-Chemistry"

GE ASAMI, Yuri; OTONARI, Kenko; IMANISHI, Miki; FUTAKI, Shiroh

"Sequence-Specific Manipulation of RNA Methylation by Engineering of an RNA Demethylase, ALKBH5"

- Chemistry of Molecular Biocatalysts -

LW "Introduction of Chemistry of Molecular Biocatalysts Laboratory"

— Molecular Biology —

[LW] "Research of Molecular Biology Laboratory"

- Chemical Biology -

LW "Create New World of Bioactive Synthetic Molecules"

— Molecular Materials Chemistry —

[LW] "Molecular Materials Chemistry"

GE ISHIHARA, Kuraudo; KAJI, Hironori "Molecular Orientation and Mobility Prediction of Organic Deposited Films by Multiscale Simulation"

- Hydrospheric Environment Analytical Chemistry -

IW "Reveal the Ocean by Using Trace Elements and Their Isotopes"

GE UEKI, Ryuta; ZHENG, Linjie; TAKANO, Shotaro; SOHRIN, Yoshiki

"Distribution of Zirconium, Hafnium, Niobium, and Tantalum in the Indian Ocean"

- Chemistry for Functionalized Surfaces -

GE ARAKI, Taisuke; SAKO, Nobuaki; SHIOYA, Nobutaka; YAJIMA, Tomoko; HASEGAWA, Takeshi

"Understanding of Physical Properties of Perfluoroalkanes by Infrared Spectroscopy Using Recrystallized Compounds"

GE SUGIMOTO, Emi; SHIOYA, Nobutaka; OKA, Takayuki; HASEGAWA, Takeshi

"Control of Crystal Orientation of Organic Semiconductors with Alkyl Side Chains in Thin Films by Low-Temperature Deposition"

— Molecular Microbial Science —

GE INOUE, Hiromu; KAWANO, Kenichi; KAWAMOTO, Jun; OGAWA, Takuya; KURIHARA, Tatsuo

"Diversity of Bacterial Extracellular Membrane Vesicles Determined by Nucleic Acid Content and the Genes Involved in Their Production"

— Polymer Materials Science —

LW "Polymer Materials Science"

-Molecular Rheology -

LW "Molecular Rheology Laboratory"

- Molecular Aggregates -

LW "Research in Molecular Aggregation Analysis Laboratory"

GE MURDEY, Richard; MATSUSHIGE, Yuko; OHASHI, Noboru; TRUONG, Minh Anh; NAKAMURA, Tomoya; WAKAMIYA, Atsushi

"Accelerated Testing of Perovskite Solar Cells"

— Particle Beam Science —

LW "Particle Beam Science Lab."

- Laser Matter Interaction Science -

III "Introduction of the Laser Matter Interaction Science Laboratory"

- Electron Microscopy and Crystal Chemistry -

w "Research Activities in Division of Electron Microscopy and Crystal Chemistry"

— Atomic and Molecular Structures —

LW "Introduction of Atomic and Molecular Structures Laboratory"

- Synthetic Organotransformation -

LW "Introduction of Synthetic Organotransformation Laboratory"

-Advanced Solid State Chemistry -

LW "Research Reports in Advanced Solid State Chemistry"

- Organometallic Chemistry -

LW "Recent Research Topics of Organometalic Chemistry Group"

- Nanophotonics -

LW "Recent Research Topics of Nanophotonics Group"

- Mathematical Bioinformatics -

LT MU, Lixuan; SONG, Jiangning; MORI, Tomoya; AKUTSU, Tatsuya "DiCleave: a Deep Learning Model for Predicting Human Dicer

Cleavage Sites"

— Bio-knowledge Engineering —

LT NGUYEN, Can Hao "Theoretical Study of Convex Clustering Algorithm"

SEMINARS

Prof AYELE, Belay Department of Plant Science, University of Manitoba, Manitoba, Canada "Insights into the Role of Jasmonate in Regulating Seed Dormancy in Wheat" 1 Jun 2023 Prof. BLACKBURN, Jeffrey National Renewable Energy Laboratory (NREL), the U.S. "Mixed-Dimensionality Nanoscale Heterojunctions for Energy Harvesting and Opto-Electronic Technologies" 24 November 2023 Assoc Prof BROERE, Daniël L. J. Institute for Sustainable and Circular Chemistry, Utrecht University, the Netherlands "Are Two Better than One? The Exploration of "Expanded Pincer" Ligands in Combination with Group 8 Metals in Hydrocarbon Activation and Homogeneous Catalysis" 10 August 2023 Prof CUMMINS, Christopher C. Department of Chemistry, Massachusetts Institute of Technology, the U.S. "Phosphorus-Element Bond-Forming Reactions from Pn to Phosphinidene Group Transfer" 15 September 2023 Prof DESTARAC, Mathias Université Toulouse 3 Paul Sabatier, France "Tailored Polyvinylamines by RAFT" 2 August 2023 Prof EMORI, Satoru Virginia Polytechnic Institute and State University, Virginia, the U.S. "Damping and Spin-Orbit Torques in Vertically Graded Fe-Ni Films' 9 May 2023 Prof FAN, Xin University of Denver, Colorado, the U.S. "Spin Current Generation in Ferromagnetic Metals" 3 March 2023 Assoc Prof FERRIER, Robert C., Jr. Michigan State University, Michigan, the U.S. "Facile Epoxide Polymerizations with Sustainable Aluminum Catalysts" 18 January 2023 Prof FINOCCHIO, Giovanni University of Messina, Italy "High Performance Spintronic Devices for Microwave Technology and Computing" 26 May 2023 Prof FRATH, Denis Laboratoire de Chimie, ENS Lyon, CNRS, France "Photoredox Control of Electron-Responsive and Conductive Supramolecular Materials Based on Viologens" 16 November 2023

Assist Prof FUKUI, Norihito

Graduate School of Engineering, Nagoya University, Nagoya, Japan "Creation of Novel π -Conjugated Molecules with the Search

Space inside the Molecular Skeleton" 27 July 2023

Dr. GALBIATI, Massimo

Institute of Agricultural Biology and Biotechnology, CNR, Milano, Italy "Deciphering the Transcriptional Regulation of Stomatal Activity" 22 November 2023

Specially Appointed Prof HIGUCHI, Yoshiki University of Hyogo, Hyogo, Japan "Elemental Cycling Strategy by Organisms" 30 October 2023

Prof HILLEBRANDS, Burkard TU Kaiserslauterun, Germany "Advances in Coherent Magnonics" 24 May 2023

Assoc Prof HINGAMP, Pascal Aix-Marseille University, France "Environmental Genomics: Bioinformatics Methods to Estimate Biodiversity from Metagenomes" 20 March 2023

Assoc Prof HINGAMP, Pascal Aix-Marseille University, France "Hands-on Introduction to Bioinformatics" 4-8, 11-12, 25 September 2023

Prof HO, Rong-Ming National Tsing Hua University, Taiwan "Well-Ordered Nanonetwork Materials from Block Copolymer Templates for Metamaterial Applications" 7 July 2023

Dr HO, Tung-Yuan Research Center for Environmental Changes, Academia Sinica, Taiwan "The Solubility and Deposition Flux of East Asian Aerosol Metals in the East China Sea: The Effects of Aeolian Transport Processes" 11 September 2023

Dr HSIEH, Chih-Chiang Research Center for Environmental Changes, Academia Sinica, Taiwan "The Contribution of East Asian Aerosol Metals in the Ocean: Sources, Transformation Processes and Deposition Fluxes" 2 October 2023

Prof HWANG, Chanyong Korea Research Institute of Standards and Science, Korea, R "Magnetic Skyrmion" 17 October 2023

Prof ILIES, Laurean RIKEN, Saitama, Japan "Catalyst Design for Selective and Efficient Reactions" 2 June 2023 Dr IMADA, Hiroshi Surface and Interface Science Laboratory, RIKEN, Wako, Japan "Developing Various Dimer Systems Based on Single-Molecule Manipulation Techniques and Evaluation of Their Optical Properties" 19 October 2023

Prof ISOBE, Hiroyuki The University of Tokyo, Tokyo, Japan "Organic Chemistry: From the Basics to the Current Style" 1 June 2023

Prof ISOBE, Hiroyuki The University of Tokyo, Tokyo, Japan "Phenine Nanocarbon Molecules" 2 June 2023

Prof ISOBE, Hiroyuki The University of Tokyo, Tokyo, Japan "Organic Chemistry: From Structure and Synthesis to Boundaries" 20 November 2023

Prof ISOBE, Hiroyuki The University of Tokyo, Tokyo, Japan "Supramolecular Science of Nanocarbon Molecules" 21 November 2023

Dr. KAKSIS, Edgar Vienna Vienna University of Technology, Austria "Scaling of Peak and Average Power in Femtosecond Ytterbium Amplifiers" 9 March 2023

Prof KIHARA, Daisuke Purdue University, the U.S. "Building and Validating Biomolecular Structure Models for cryo-EM Maps Using Deep Learning" 28 June 2023

Prof KOBAYASHI, Toshihide Centre National de la Recherche Scientifique (CNRS), France "Regulatory Proteins for the Asymmetric Distribution of Sphingomyelin" 25 May 2023

Prof LIAN, Tianquan Department of Chemistry, Emory University, Georgia, the U.S. "Structure and Dynamics at Metal Electrode/Electrolyte Interface Probed by Insitu Electrochemical Surface Enhanced/Selective Vibrational Spectroscopy" 8 May 2023

Prof. LIN, Hao-Wu National Tsing Hua University, Taiwan "Perovskite Optoelectronic Devices: Solar Cells and Beyond" 5 July 2023

Prof LIU, Hongbin The Hong Kong University of Science and Technology, China P.R. "Diversity and adaptation of Synechococcus in Estuarine Waters" 20 January 2023

Prof MARGETIĆ, Davor Ruđer Bošković Institute, Croatia "The Reactivity of Guanidine Substituted Furans and Pyrroles in Cycloaddition Reactions" 11 September 2023 Prof MARTIN-VACA, Blanca Paul Sabatier University and Centre national de la Recherche Scientifique, France "Cooperative Catalysis with Pd and Pt Pincer Complexes" 3 March 2023

Prof MINDIOLA, Daniel J.

Department of Chemistry, University of Pennsylvania, the U.S. "New Developments in Low-Valent and Early Transition Metal Ions, Metal-Ligand Multiple Bonds, and Catalytic Reactions Involving Methane" 11 July 2023

Prof NAKAI, Madoka Tokyo University of Agricultural and Technology, Tokyo, Japan "Frontiers of Insect Virus Research Contributing to Pesticide Reduction and Training the Next Generation of Researchers" 27 December 2023

Prof NAKANO, Ken *et al.* Yokohama National University, Yokohama, Japan "SRT Basic Seminar (Series of 8 Sessions)" 6-30 July 2023

Prof NGUYEN, Thuc-Quyen Department of Chemistry & Biochemistry, University of California Santa Barbara, California, the U.S. "Designing Organic Semiconductors for Energy Generation and Infrared Sensing" 11 December 2023

Dr NISHIMURA, Masaki Technology Research Institute of Osaka Prefecture, Osaka, Japan "A Researcher's Life in Public Testing Research Institute: between Industry, Technology, and Science" 26 May 2023

Prof NOMURA, Nobuhiko Faculty of Life and Environmental Sciences, University of Tsukuba, Ibaraki, Japan "Emergence of Bacterial Community Formation and Sociality" 30 January 2023

Prof OGASAWARA, Masamichi Department of Natural Science, Graduate School of Science and Technology, Tokushima University, Tokushima, Japan "Enantioselective Catalytic Synthesis of Chiral Transition Metal Complexes" 27 January 2023

Dr. OGAWA, Satoshi Botany and Plant Sciences Faculty, University of California, Riverside, California, the U.S. "Molecular Basis for Host Tropism in Orobanchaceae Parasitic Plants" 21 November 2023

Prof. POPMINTCHEV, Tenio University of California San Diego, the U.S. "Quantum Optics Meets Strong Field Physics: Novel Regimes of Coherent X-Ray Generation with Strong Electron Correlation Dynamics and Attosecond Rabi Oscillations" 12 December 2023

Prof RIVARD, Eric Department of Chemistry, University of Alberta, Alberta, Canada "Frustrated Lewis Pair (FLP) Chelation for Main Group Materials Synthesis" 8 March 2023 Assist Prof RUBIO, Vicente Centro Nacional de Biotecnologia, CSIC, Madrid, Spain "Dangerous Liaisons: COP1 and DET1 Regulatory Loops in Controlling Plant Development" 12 October 2023

Assist Prof SADIQ, Nausheen W. Department of Chemistry, Mount Royal University, Canada "Evaluating Risk to Human Health Associated with Microplastics, Contaminated Soils, Waters and a Variety of Food Samples at the Elemental Level Using ICP-MS" 9 March 2023

Prof SAITO Hiroaki Atmosphere and Ocean Research Institute, The University of Tokyo, Tokyo, Japan "Prochlorococcus in the Indian Ocean" 20 January 2023

Assoc Prof SAKAI, Munetoshi Ibaraki University, Ibaraki, Japan "Functional Evaluation Method for Dynamic Wettability on Solid Surfaces" 28 August 2023

Assoc Prof SARAKONSRI, Thapanee Department of Chemistry, Faculty of Science, Chiang Mai University, Thailand "Enhanced Electrochemical Performance of Nanocomposite Anode Materials with High Energy Density, Ultrafast-Charging and Stable Cycling for High- Efficiency Li-Ion Batteries"

Prof. SASAMORI, Takahiro University of Tsukuba, Ibaragi, Japan "Introduction of Single Crystal X-ray Diffraction Analysis -Key Points to Consider When Facing Analytical Challenges-" 14 June 2023

Dr SATO, Yuya Environmental Management Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan "Emergence of Unique Biological Functions Triggered by Microbe-Driven Interspecific Relationships" 17 November 2023

Prof SCHELER, Ulrich Leibniz-Institut für Polymerforschung Dresden e. V., Germany "NMR Studies for Complex Polymer Materials" 30 October 2023

Dr. SHI, Dongbo Institute for Biochemistry and Biology, University of Potsdam, Potsdam-Golm, Germany "Identification of Cambium Stem Cells and Their Dynamics" 26 July 2023

Prof SUNAGAWA, Shinichi Institute of Microbiology and Swiss

5 June 2023

Institute of Microbiology and Swiss Institute of Bioinformatics ETH Zurich, Germany "The Ocean Microbiome as a Treasure Trove for Novel Taxa, Enzymes and Bioactive Compounds" 25 July 2023

Prof TABOR, Alethea Department of Chemistry, University College of London, the U.K. "Liposome-Based Theragnostic Nanoparticles for Cancer Imaging, Nucleic Acid and Drug Delivery" 5 September 2023 Lect TASHIRO, Yosuke

College of Engineering, Shizuoka University, Shizuoka, Japan "Diversity of Bacterial Membrane Vesicles and the Molecular Basis for the Regulation of Vesicle Production" 17 May 2023

Prof TCHORZEWSKI, Marek

Department of Molecular Biology, Institute of Biological Sciences, Maria Curie-Sklodowska University, Poland "Ribosome: A Multifaceted Nano-Machine" 28 June 2023

CNRS Research Fellow THILI, Anis University of Lyon 1, France "Valorization of Greenhouse Gases: CO₂, SF₆ and Beyond" 30 October 2023

Prof TOKUYAMA, Hidetoshi Tohoku University, Miyagi, Japan "Novel Oxygen Oxidation Reaction and Unprotected Peptide Dimerization and its Application to Alkaloid Synthesis" 21 November 2023

Assist Prof TSUCHIDO, Yoshitaka Faculty of Science Division I, Tokyo University of Science, Tokyo, Japan "Synthesis and Functions of Cyclic π-Conjugated Compounds via Macrocyclic Gold Complexes" 26 May 2023

Prof VAZQUEZ, Manuel Spanish National Council for Research, Spain "Cylindrical Magnetic Micro and Nanowires: from Topology Effects of Curvature to Sensing Applications" 26 May 2023

Prof WATERMAN, Rory University of Vermont, California, the U.S. "Metal-Catalyzed Routes to Low-Valent Main Group Fragments" 8 May 2023

Prof WECKWERTH, Wolfram University of Vienna, Austria "Multiomics, AI and Data-Driven Inverse Modelling - from Environmental Sciences to Molecular Medicine" 16 November 2023

Prof WEITZ, Joshua University of Maryland, the U.S. "Marine Viral Dynamics: Lessons from an Imperfect Predator" 7 July 2023

Prof WIRTH, Thomas Cardiff University, the U.K. "New Opportunities for Flow Electrochemistry" 27 September 2023

Prof YAMAKOSHI, Yoko Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich, Switzerland "Water-Soluble Fullerene Materials and Their Photosensitising Activity" 5 December 2023

Prof. ZHANG, Deqing Institute of Chemistry, Chinese Academy of Sciences, China P.R. "New Conjugated Molecules for Organic and Polymeric Semiconductors" 11 December 2023

MEETINGS AND SYMPOSIA

International Workshop on Bioinformatics and Systems Biology (IBSB) Organized by MAMITSUKA, Hiroshi 17-21 January 2023 (Berlin, Germany)

Future Drug Discovery Empowered by Chemical Biology Organized by UESUGI, Motonari 21-22 February 2023 (Nara, Japan)

ACBI 2023 Toba Meeting Organized by UESUGI, Motonari 22-24 February 2023 (Mie, Japan)

Spin-RNJ Symposium 2022 Organized by ONO, Teruo 20 March 2023 (Kyoto, Japan)

NII Shonan Seminar, NO.179 Computational Metabolomics and Machine Learning Organized by MAMITSUKA, Hiroshi 8-11 May 2023 (Kanagawa, Japan)

The 19th Akabori Conference

Organized by FUTAKI, Shiroh 16-20 May 2023 (Shiga, Japan)

10th Pacific Symposium on Radical Chemistry (PSRC-10) Organized by YAMAGO, Shigeru 4-9 June 2023 (Kyoto, Japan)

The 1st Kyoto-SKKU Workshop Organized by WAKAMIYA, Atsushi 5 June 2023 (Kyoto, Japan)

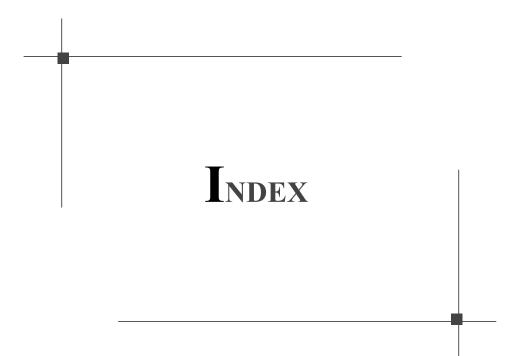
RURSS Unit Meeting #1 in 2023: Toward Starting Over of PFAS Science Organized by HASEGAWA, Takeshi 30 June 2023 (Kyoto, Japan)

Frontiers of Disease Informatics (Workshop in IIBMP 2023) Organized by AKUTSU, Tatsuya 8 September 2023 (Kashiwa, Japan)

1st Expert Committee on Mid-Infrared Laser Technology Organized by TOKITA, Shigeki 27 September 2023 (Kyoto, Japan)

The First Perovskite International Research Collaboration Center (PIRCC) Workshop Organized by WAKAMIYA, Atsushi 3 October 2023 (Kyoto, Japan) The 2nd Seminar on International Core-to-Core Project on Nano Carbon Device Science at Kyoto Organized by YAMAGO, Shigeru; KAJI, Hironori; HIROSE, Takashi 4-6 October 2023 (Kyoto, Japan)

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