

ICR ANNUAL REPORT

2020

Volume 27

Institute for Chemical Research
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.



■ <http://www.kikin.kyoto-u.ac.jp/contribution/chemical/>

**ICR
ANNUAL
REPORT
2020**



**Institute for Chemical Research
Kyoto University**
Volume 27



Preface

The Institute for Chemical Research (ICR) was founded in 1926 as the first research institute of Kyoto University. Its founding vision was “excel in the investigation of the basic principles of chemistry and their applications.” ICR is a successor to the Specialized Center for Chemical Research established at the College of Science of Kyoto Imperial University in 1915 for the study of a special medicinal substance called “Salvarsan,” that is arsphenamine. Ever since, ICR has continuously carried out outstanding research and flourished as a large-scale organization. We have 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). Currently, almost 120 faculty members, 210 graduate students, and 60 researchers are engaged in research activities in 30 laboratories directed by fulltime professors and 5 laboratories supervised by visiting professors. These laboratories are affiliated as a “cooperative lab” with graduate schools covering a broad range of fields such as science, engineering, agriculture, pharmaceutical sciences, medicine, and informatics.

Based on the founding vision, ICR has encompassed a wide range of scientific disciplines, including physics, biology, and informatics, as well as chemistry. ICR members are spearheading cutting-edge research and yielding groundbreaking results in their special fields. Some of the research achievements last year are as follows: 1) *Jitter-free Electron Pulses Directly Accelerated by an Intense Laser Beam and Their Application*; 2) *Discovery of Self-Assembling Small Molecules as Vaccine Adjuvants*; 3) *Biogeography of Marine Giant Viruses Reveals Their Interplay with Eukaryotes and Ecological Functions*; 4) *Observation of Superconducting Diode Effect*; 5) *Organic Light Emitters Exhibiting Very Fast Reverse Intersystem Crossing*; 6) *Modifying Angular and Polarization Selection Rules of High-order Harmonics by Controlling Electron Trajectories in k -Space*; 7) *Additive-Free Conversion of Internal Alkynes by Phosphanylaluminanes*. Some other topics were also presented in the 120th ICR Annual Symposium on December 11, 2020.

The legacy of our founding philosophy continues today and describes the essence of our research activities. With the founding vision in mind, we have entrusted our scientists with the responsibility of choosing research topics

within advanced chemistry-related fields. Thus, ICR members are actively involved in interdisciplinary research projects, creating new knowledge and contributing to the future of materials-related fields. One of our major new challenges is the design of ecologically sustainable smart materials. Our institute is collaborating with other research institutions inside and outside Kyoto University as a key member of the following projects/organizations: *MEXT Inter-University Collaborative Project “Integrated Consortium on Chemical Synthesis”* including four core research institutions, *Kyoto University Research Coordination Alliance* including 19 research institutes/centers of Kyoto University, *MEXT-supported “under-one-roof” Joint Project* on bio-inspired smart materials in Uji Campus, and *Uji-Campus Base of Equipment Support* for reinforcing research infrastructure. We also promote international collaboration with overseas universities/institutions (with 68 official international collaboration agreements). On the basis of our strong global activity in chemistry-oriented fields, ICR was newly certified as an *International Joint Usage/Research Center* by MEXT in 2018 and approved by Kyoto University in 2019 to establish an *On-site Laboratory*, the “*Kyoto University Shanghai Lab*” in Shanghai, China under the Designated National University program (MEXT). To foster and secure young researchers through these activities, we have initiated diverse research and graduate education programs, including an in-house annual grant system, “*ICR Grant for Promoting Integrated Research*.” These collaborative achievements ensure that our institute serves as a global research core in chemistry-oriented fields.

In recent years, many global-scale problems have become apparent. Science and technology must play a large role to help society mitigate and overcome disasters such as the new coronavirus as well as longer term issues such as climate change and environmental pollution. With keywords of “Diversity” and “One Team” together with the founding vision, ICR continues to strive to answer those challenges, promoting a multidisciplinary, chemistry-related community, and deepening science and technology for a sustainable society. We hope this Annual Report will serve to update you on the progress of our research activities and globalization. Finally, we appreciate your continued encouragement and support.

January 2021

A handwritten signature in black ink, appearing to read 'Y. Tsujii'.

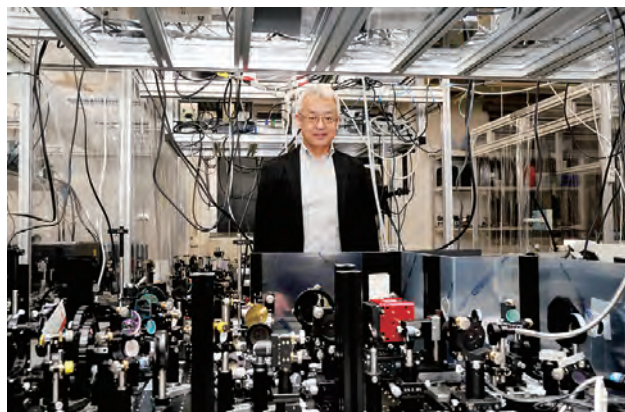
TSUJII, Yoshinobu
Director

ICR News 2020

Grant-in-Aid for Specially Promoted Research Title of Project: Fusing Nanomaterials and Strong Electric Field Nonlinear Optics for New Advances in Photonics

■ Prof KANEMITSU, Yoshihiko

Based on its expertise in optics and nanoscience, the laboratory of Professor Yoshihiko Kanemitsu has been studying the optical properties of new solid crystals and nanomaterials. Following its previous work (funding sources include Grant-in-Aid for Scientific Research, Kakenhi, in 2008, the SEI Group CSR Foundation in 2011, and Strategic Basic Research Program Grants, JST-CREST, in 2011 and 2016.), the Kanemitsu group started a new project in April 2019. The project involves the fabrication of nanomaterials and crystal structures with unique electronic properties. Applying ultrafast laser spectroscopy with a set electric field phase to these materials will lead to new strong electro-optics and quantum photonics technologies. The key words of the research are “light phase” and “electron phase”. By manipulating the movement of electrons in matter with a laser electric field, new nonlinear optical phenomena are expected. We appreciate your support.



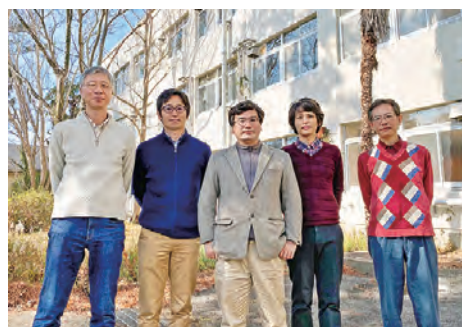
Challenge for the Complete Utilization of Solar Energy

■ Assoc Prof SAKAMOTO, Masanori

Sun is the most important energy source supporting life on Earth and human activities. However, solar light in the IR region, which makes up almost half of all solar energy, has been untapped by neither natural photosynthesis nor artificial photo-energy conversion systems. The development of technology, which allows us to utilize the energy of solar light in the IR region, will provide a vast energy source for human society.

The utilization of IR light realizes energy production in harmony with nature in the truest sense. Because nature does not utilize the IR light as an energy source, utilization of IR energy does not compete with natural photosynthesis or conventional artificial photo-energy conversion systems like photovoltaics. Furthermore, the invisibility of IR light paves the way to the development of unique devices such as transparent photovoltaic glass which can be applied to the windows of the skyscrapers.

The project team of Masanori Sakamoto is challenging the utilization of untapped IR lights from the viewpoint of developing both a new field of science and the next-generation solar industry. Through the interdisciplinary collaboration with Prof. Koji Tanaka (iCems, Kyoto University), Katsuaki Kobayashi (Osaka City University), Mitsuhiro Arisawa (Osaka University), Akira Yamakata (Toyota Institute of Technology), and Akihiro Furube (Tokushima University), we will construct new scientific fields realizing the untrodden complete utilization of solar energy.



ICR's Supercomputer System Renewed

■ Prof OGATA, Hiroyuki

The supercomputer system of ICR has been helping computational studies in broad areas of chemistry and biology, and continuously performing its special mission to provide biological database services through GenomeNet since 1992. The system is designed to serve not only experts in computational studies but also experimental researchers by supplying an array of user-friendly software and databases. In January 2020, the supercomputer system has experienced its sixth replacement. The renewed system is composed of two nodes of shared memory machines (48 TB memory and 1152 CPU cores in total) and a computer cluster (142 nodes including 18 GPU nodes, 5680 CPU cores in total) connected through a fast network (100 Gbps InfiniBand). Its storage system comprises a distributed file system (6.1 PB) and a network file system (2.3 PB). Finally, the system provides and maintains KEGG, a prominent database in life science developed in ICR since 1995.



The shared memory system and the high-performance computer cluster.



The robust network file system that stores user data and the databases of GenomeNet.



The distributed file system allowing high-speed file access is used for big data computations.

News from International Public Relations

ICR Hosted Three Student Awardees from Mongolia

On the occasion of *KAPLAT Talent-Spot 2019 Ulaanbaatar* held in September 2019, KAPLAT Travel Award was presented to 3 top-performing students out of 16 student candidates from Mongolia. In January 2020, the awardees, all of whom were coincidentally from the National University of Mongolia, 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, and the best presentation award went to Manchir Tserendagva. She eventually joined an ICR laboratory as a MEXT scholar and now pursues a Master's degree from Kyoto University.



JST Sakura Science Plan

Sakura Science Plan is an international exchange program of JST, which provides young Asian students with science and technology experience in Japan. With the support of this project, ICR invited four undergraduate students from the National University of Mongolia in February 2020. They spent one week in the lab of their choice and had opportunities to do experiments with leading researchers at state-of-the-art research facilities, to which they have little or no access back home. These experiences triggered their motivation to study at Kyoto University for an advanced degree in the near future.



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



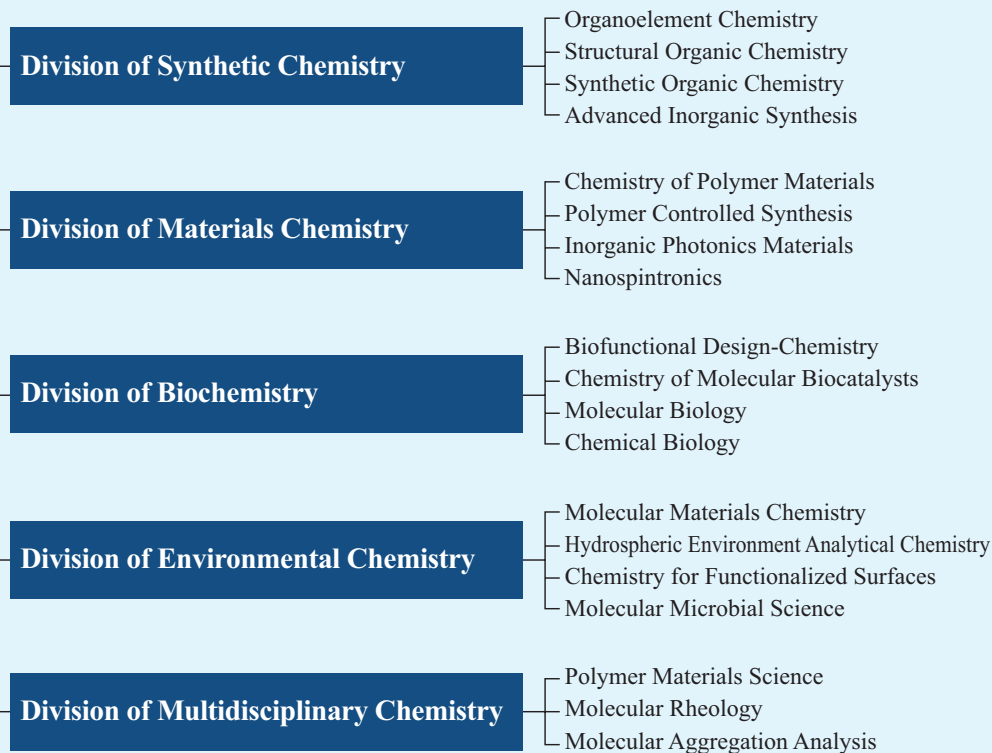
ORGANIZATION

Institute for Chemical Research

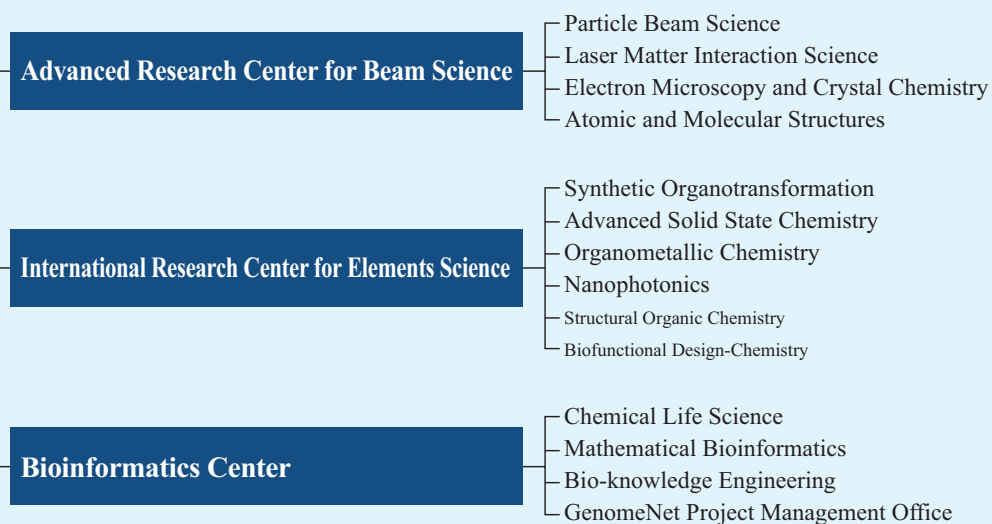
5 Divisions and 3 Centers

Laboratories

Research Divisions

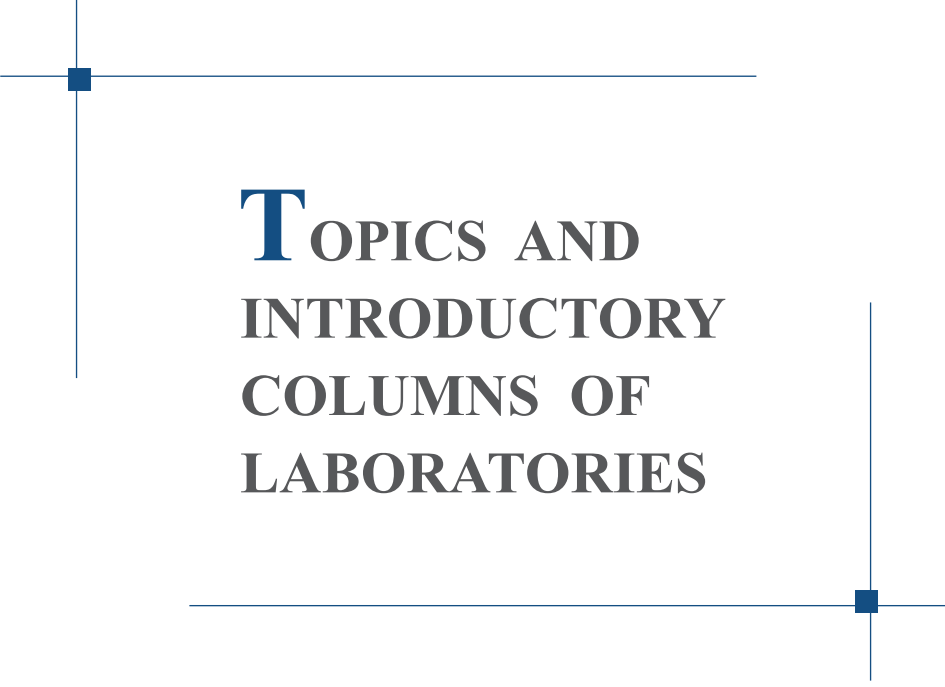


Research Centers



Visiting Divisions

- International Joint Usage/Research Center
- Supercomputer System
- Low Temperature Laboratory



TOPICS AND
INTRODUCTORY
COLUMNS OF
LABORATORIES

Division of Synthetic Chemistry – Organoelement Chemistry –

http://oec.kuicr.kyoto-u.ac.jp/~tokitohlab/index_e.html



Prof

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Assoc Prof

MIZUHATA, Yoshiyuki
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Assist Prof

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JUN-I, Yuta (D2)

OSHIRO, Taku (D2)

TSUJI, Shingo (D2)

GARCIA, Julius (D2)

HONJO, Kazuma (M2)

SASAYAMA, Ryuto (M2)

YASUI, Yuji (M2)

YANG, Yi (M2)

KANDA, Kazuaki (M1)

SUITO, Taisuke (M1)

Scope of Research

Organic chemistry has mainly developed with the use of second-row elements such as carbon, oxygen, and nitrogen, while the synthesis and isolation of the heavier congeners of typical organic molecules as stable compounds has been a dream for organic chemists. Our main research interest is the elucidation of the similarities and differences in structures and reactivities between organic compounds and the corresponding heavier congeners. These studies are interesting and important from the standpoints of fundamental chemistry, and open the way to the more extensive application of main group chemistry.

KEYWORDS

Steric Protection
Kinetic Stabilization
Low-coordinated Species
Heteroatom
Transition Metal Complexes



Selected Publications

Mizuhata, Y.; Fujimori, S.; Sasamori, T.; Tokitoh, N., Germanbenzylpotassium: A Germanium Analogue of a Phenyl Anion, *Angew. Chem. Int. Ed.*, **56**, 4588-4592 (2017).

Fujimori, S.; Mizuhata, Y.; Tokitoh, N., Stannabenzenylpotassium: The First Isolable Tin-containing Benzene Derivative, *Chem. Eur. J.*, **24**, 17039-17045 (2018).

Fujimori, S.; Mizuhata, Y.; Tokitoh, N., A Mixed-anion System Consisting of a Germyl Anion and Anions Delocalized on Conjugated Carbon Ring Skeletons, *Chem. Eur. J.*, **25**, 6284-6289 (2019).

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Kunzmann, R.; Omatu, Y.; Schnakenburg, G.; Espinosa Ferao, A.; Yanagisawa, T.; Tokitoh, N.; Streubel, R., A Synthetic Equivalent for Unknown 1,3-Zwitterions? – A K/OR Phosphinidenoid Complex with an Additional Si–Cl Function, *Chem. Commun.*, **56**, 3899-3902 (2020).

Division of Synthetic Chemistry – Structural Organic Chemistry –

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



Prof
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Assoc Prof
HIROSE, Takashi
(D Eng)



Assist Prof
HASHIKAWA, Yoshifumi
(D Eng)



PD
ZHANG, Sheng
(Ph D)

Students

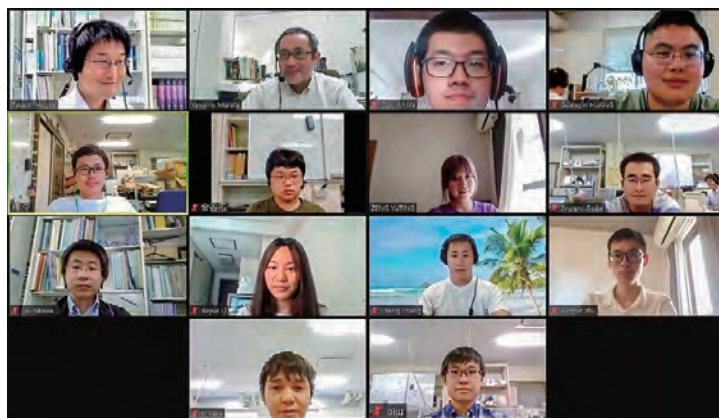
HUANG, Guanglin (D2)	ZHU, Xiaotan (M1)	SADAI, Shumpei (UG)
KANAYA, Taku (M2)	GU, Jiajian (M1)	MIYAKE, Yuya (UG)
LI, Hui (M2)	ZENG, Yuting (RS)	OKUSHIMA, Ryota (UG)
LI, Jiayue (M1)	LIU, Zhibo (RS)	

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 C_{60} and C_{70} , 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	Endohedral Fullerenes
Functional Materials	Helical Structures
Radical Species	



Selected Publications

Hashikawa, Y.; Fushino, T.; Murata, Y., Double-Holed Fullerenes, *J. Am. Chem. Soc.*, **142**, 20572-20576 (2020).
Hashikawa, Y.; Murata, Y., Cation Recognition on a Fullerene-Based Macrocyclic, *Chem. Sci.*, **11**, 12428-12435 (2020).
Hashikawa, Y.; Hasegawa, S.; Murata, Y., Precise Fixation of an NO Molecule inside Carbon Nanopores: A Long-Range Electron-Nuclear Interaction, *Angew. Chem. Int. Ed.* (in press).
Hashikawa, Y.; Okamoto, S.; Murata, Y., Organophosphorus Zwitterions Engaged in a Conjugated Macrocyclic on Fullerene, *Commun. Chem.*, **3**, 90 (2020).
Kubo, H.; Shimizu, D.; Hirose, T.; Matsuda, K., Circularly Polarized Luminescence Designed from Molecular Orbitals: A Figure-Eight-Shaped [5]Helicene Dimer with D_2 Symmetry, *Org. Lett.*, **22**, 9276-9281 (2020).

Organophosphorus Zwitterions Engaged in a Conjugated Macrocycle on Fullerene

Organophosphorus zwitterions are one of the most important but elusive intermediates for carbon–carbon bond formation in synthetic chemistry and biology. However, a lack of isolated examples due to their lability has hampered in-depth understanding of structures and their reaction mechanisms. In this study, we crystallographically reveal the solid-state structure of a phosha-Michael adduct engaged in a cage-opened C_{60} skeleton, which is formed as a kinetic product. This compound exhibits dark brown colour in solution with an intense absorption band that extends to 1,000 nm, reflecting intramolecular charge transfer transitions. From the 1,2-dicarbonyl moiety on the conjugated orifice, β -oxo-phosphorus ylide is formed as a thermodynamic product. The reaction mechanism that has long been disputed is examined by experimental and theoretical studies, showing a pathway which includes an S_N2 reaction as a key step instead of the hitherto considered carbene pathway.

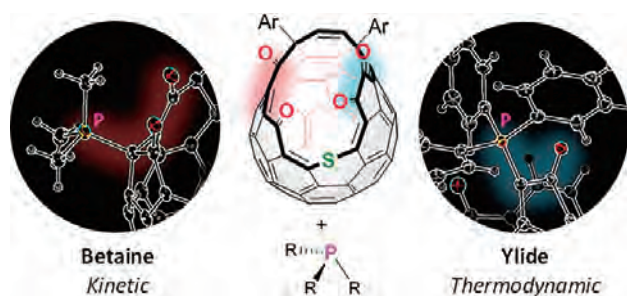


Figure 1. Organophosphorus zwitterions on a cage-opened fullerene derivative.

Double-Holed Fullerenes

Fully-fused caged nanocarbons with multiple orifices are segmental structures of porous carbon frameworks long envisioned as synthetic targets of interest. Conventional bottom-up approaches, however, could not overcome the high strain energies required for graphitic precursors to be rounded up. We demonstrated a top-down approach to produce fully fused carbon nanoelbows as double-holed fullerenes derived from strained C_{60} . The concise one-pot synthesis featuring unique selectivity enabled the isolation of six compounds, while orifice sizes were modifiable from 8- to 12-membered rings and vice versa. The crystallographic analysis confirmed their elbow-shaped structures with different curvatures. Within the crystal, cylindrical nanoporous arrangement were found with the inclusion of solvent guests, reminiscent of hypothetical fullerene sponges.

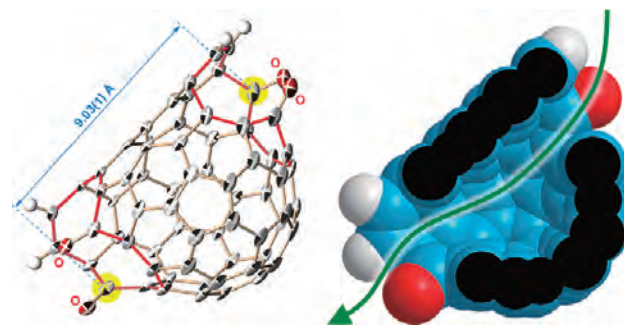


Figure 2. A double-holed fullerene.

Circularly Polarized Luminescence Designed from Molecular Orbitals: A Figure-Eight-Shaped [5]Helicene Dimer with D_2 Symmetry

The shape and symmetry of molecular orbitals determine the photophysical properties of molecules. Although many chiral molecules exhibiting circularly polarized luminescence (CPL) have been reported, few general methods are known to achieve large dissymmetry factor for CPL (g_{CPL}). To maximize the g_{CPL} values, transition electric dipole moment μ and transition magnetic dipole moment m are required to be parallel and of the same magnitude. Regarding the former criterion, from the viewpoint of the group theory, we noticed that D_2 symmetry is the only point group where the directions of μ and m vectors are always parallel for all electronic transitions. We synthesized and demonstrated that a figure-of-eight shaped [5]helicene dimer with the D_2 -symmetry has excellent chiroptical properties ($\Phi_f = 0.08$, $|g_{CPL}| = 1.5 \times 10^{-2}$), which is attributed to the parallel arrangement of μ and m as well as a good $|\mu|/|m|$ ratio.

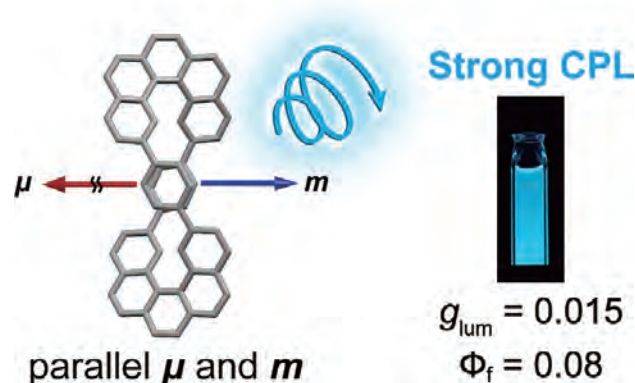


Figure 3. A CPL-active [5]helicene dimer with the D_2 symmetry.

Division of Synthetic Chemistry

– Synthetic Organic Chemistry –

<http://www.fos.kuicr.kyoto-u.ac.jp/EnglishTop/English.top.html>



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XING, Yongning (D3)

NINOMIYA, Ryo (D3)

HASHIMOTO, Hisashi (D2)

EMI, Ryota (M2)

SHIGEMATSU, Hajime (M2)

FUJIMURA, Kouki (M2)

TANIGAKI, Yusuke (M1)

UJI, Akihito (UG)

Scope of Research

The research interests of this laboratory include the development of advanced molecular transformation, total synthesis of biologically active products, and molecular recognition. Programs are active in the following areas: 1) asymmetric alkylation of carbonyl compounds based on “memory of chirality”, 2) organocatalysis for fine organic syntheses, 3) synthesis of unusual amino acids and nitrogen heterocycles, 4) regioselective functionalization of carbohydrates, and 5) the structural and functional investigation of heterochiral oligomers.

KEYWORDS

Site-Selective Functionalization
Molecular Recognition
Organocatalysis
Dynamic Chirality
Unusual Amino Acid

Selected Publications

Kawabata, T.; Moriyama, K.; Kawakami, S.; Tsubaki, K., Powdered KOH in DMSO: An Efficient Base for Asymmetric Cyclization via Memory of Chirality at Ambient Temperature, *J. Am. Chem. Soc.*, **130**, 4153-4157 (2008).

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Imayoshi, A.; Lakshmi, B.; Ueda, Y.; Yoshimura, T.; Matayoshi, A.; Furuta, T.; Kawabata, T., Enantioselective Preparation of Mechanically Planar Chiral Rotaxanes by Kinetic Resolution Strategy, *Nat. Commun.*, **12**, 404 (2021).

Enantioselective Preparation of Mechanically Planar Chiral Rotaxanes by Kinetic Resolution Strategy

The field of asymmetric synthesis is becoming a mature science. On the other hand, asymmetric synthesis of chiral mechanically interlocked molecules such as mechanically planar chiral rotaxanes and topologically chiral catenanes (Figure 1) has been rather unexplored, and their highly enantioselective synthesis has been a long-standing dream in organic synthesis. Here we report our efforts toward this goal. The strategy relies on kinetic resolution of racemic mechanically planar chiral rotaxanes by catalytic asymmetric acylation of the hydroxy group (Figure 2a). An expected problem was determining how can such remote asymmetric induction be achieved? Methods for acylative kinetic resolution of racemic alcohols have been extensively investigated, and efficient discrimination of chirality

of substrate alcohols has been achieved when the reacting center (OH) in the substrate is close to the chiral center (Figure 2b). On the other hand, discrimination of the chirality of the substrate by acylation of the hydroxy group located at the edge of the huge mechanical interlocked molecule may not be readily achievable (Figure 2a). However, use of our original catalyst accomplished the objective. Kinetic resolution of the racemic rotaxane **1** was performed with catalyst **2** via remote asymmetric acylation of a hydroxy group in the axis component to successfully provide an unreacted enantiomer in up to >99.9% ee in 29% yield (Figure 3) (The theoretical maximum yield of kinetic resolution of racemate is 50%). While the rotaxane molecule is expected to have conformational complexity, catalyst **2** enabled to discriminate the mechanical chirality of the rotaxanes efficiently with the selectivity factors in up to 16 (*Nat. Commun.* **2021**, 12, 404).

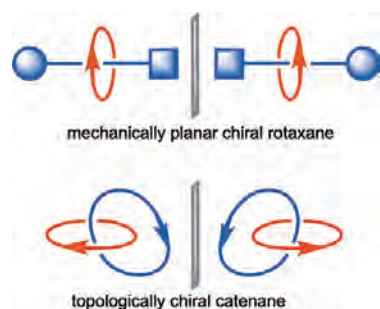


Figure 1

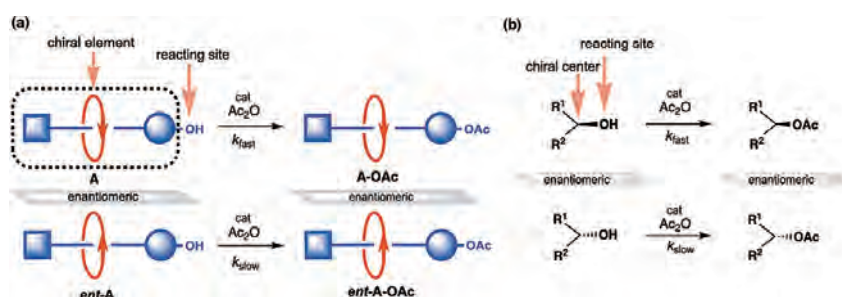


Figure 2

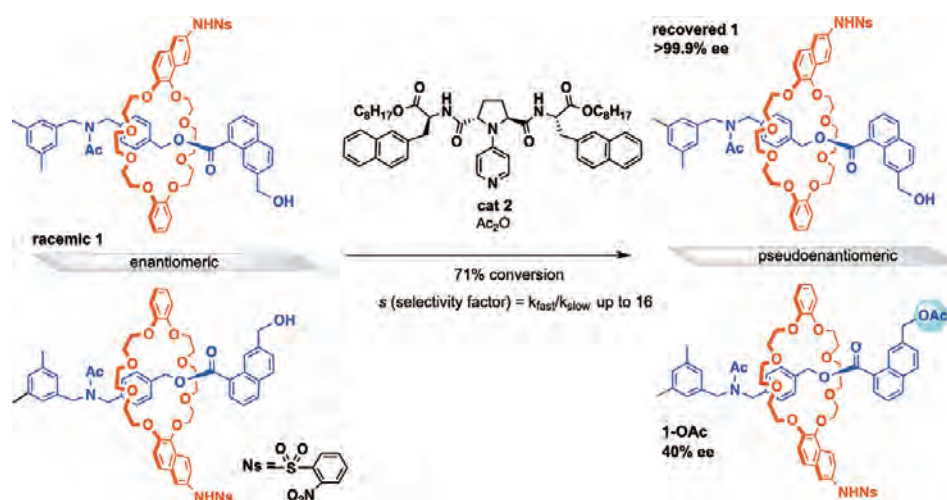


Figure 3

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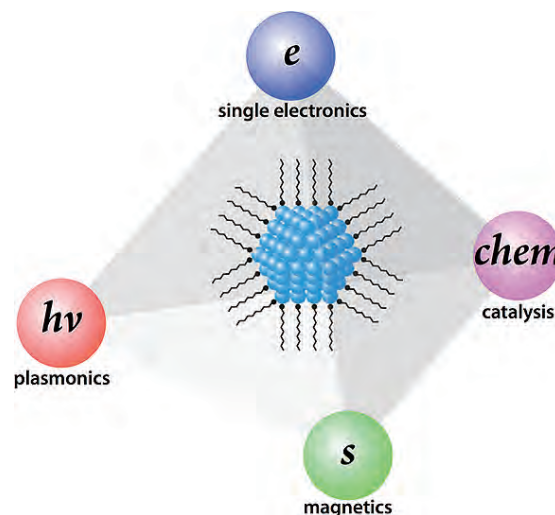
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Scope of Research

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 Nanoparticles Single Electronics Plasmonics
Nanocomposite Magnet Photocatalysts



Selected Publications

Saruyama, M.; Kim, S.; Nishino, T.; Sakamoto, M.; Haruta, M.; Kurata, H.; Akiyama, S.; Yamada, T.; Domen, K.; Teranishi, T., Phase-Segregated NiP_x@FeP_yO_z Core@Shell Nanoparticles: Ready-to-Use Nanocatalysts for Electro- and Photo-Catalytic Water Oxidation through *in-situ* Activation by Structural Transformation and Spontaneous Ligand Removal, *Chem. Sci.*, **9**, 4830-4836 (2018).

Lian, Z.; Sakamoto, M.; Matsunaga, H.; Vequizo, J. J. M.; Yamakata, A.; Haruta, M.; Kurata, H.; Teranishi, T., Near Infrared Light Induced Plasmonic Hot Hole Transfer at a Nano-Heterointerface, *Nat. Commun.*, **9**, 2314 (2018).

Eguchi, D.; Sakamoto, M.; Teranishi, T., Ligand Effect on the Catalytic Activity of Gold Clusters in the Electrochemical Hydrogen Evolution Reaction, *Chem. Sci.*, **9**, 261-265 (2018).

Number of Surface-attached Acceptors on a Quantum Dot Impacts Energy Transfer and Photon Upconversion Efficiencies

Photon upconversion, which converts low-energy photons into high-energy photons, is attractive for various applications including solar energy conversion, bioimaging, and optogenetics. Compared with upconversion using lanthanide-based nanocrystals, triplet–triplet annihilation upconversion (TTA-UC) can occur under a relatively low light flux comparable to that of sunlight. Quantum dots (QDs) are excellent light-harvesting materials that efficiently absorb light ranging from the ultraviolet to the infrared region. The quantum yield of triplet–triplet energy transfer (TTET) from QDs to suitable organic molecules has been demonstrated to reach almost 100%. Moreover, the energy loss induced by singlet–triplet energy gaps (ΔE_{ST}) can be decreased by the characteristic small singlet–triplet splitting ($\Delta E_{ST} < 15$ mV) of QDs. Therefore, composites of QDs and organic molecules have emerged as an ideal TTA-UC system that can potentially reach higher efficiency. However, the UC efficiency of QD-molecular composites is still lower than that reported for a molecular system. The tailored approach promoting the UC efficiency using QDs has been required. Herein, we discovered that the number of acceptor molecules (n) on a single QD dictates the efficiencies of triplet–triplet energy transfer (TTET) and TTA-UC. Systematic investigation of different types of QDs (CdSe, CdTe) coordinated with precisely determined numbers of perylene-3-carboxylic acid (Pe) ligands revealed that both TTET and TTA-UC efficiencies are determined by the number of Pe on a QD. Based on our results, we demonstrated that the intrinsic TTET efficiency (Φ_{TTET}/n) independent of the number of acceptor molecules is a good evaluation guide of TTA-UC systems. The proper choice of QDs and acceptors providing both sufficient free energy change for TTET and high n are important to achieve efficient TTA-UC.

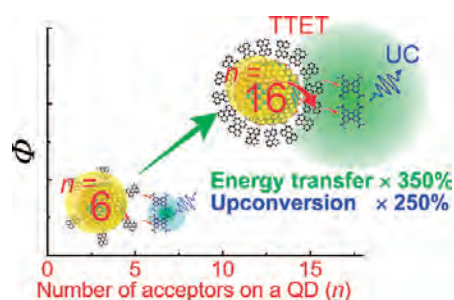


Figure 1. Illustration of triplet–triplet annihilation upconversion (TTA-UC) using QD-molecular composites. The number of molecules on a QD determines the efficiencies of triplet–triplet energy transfer (TTET) and TTA-UC. (Adapted with permission from ACS Photonics 2020, 7, 1876-1884. Copyright 2020 American Chemical Society.)

Self-activated Rh–Zr Mixed Oxide as a Nonhazardous Cocatalyst for Photocatalytic Hydrogen Evolution

Photocatalytic water splitting is a desirable technology for sustainable hydrogen production. Various kinds of photocatalysts have been developed for effective utilization of solar energy. In addition, developing cocatalysts for photocatalysis is also indispensable for improving photocatalytic activity; this is because the cocatalysts can promote extraction of excited charges from the photocatalysts and reduce the activation energy of the water splitting reaction. Though RhCrO_x is commonly used because of their excellent activity, long-time photo-irradiation causes elution of Cr(VI) ions, resulting in not only decreased activity but also environmental damage and health hazards. Here we demonstrate that a Rh–Zr mixed oxide works as an efficient cocatalyst for hydrogen evolution. Impregnation of Zr and Rh complexes (Zr/Rh = 5 wt/wt%) formed RhZrO_x mixed oxide cocatalyst particles on Al-doped SrTiO_3 , which showed 31 times higher photocatalytic water splitting activity than a RhO_x cocatalyst. X-ray photoelectron spectroscopy revealed that the dissociation of Cl^- ions from preformed Rh–Cl–Zr–O solid led to formation of the active phase of RhZrO_x . Electrochemical measurements showed that addition of Zr suppresses not only the ORR, but also the HER of Rh. This fact determines the proper weight ratio of Zr/Rh (= 5) in RhZrO_x for water reduction reaction. Additional CoO_x loading as a water oxidation cocatalyst further improved the activity by 120%, resulting in an apparent quantum yield of ca. 33% at 365 nm and a good durability in at least 60 h. This novel nonhazardous Zr-based cocatalyst will be useful for large-scale solar-hydrogen production.

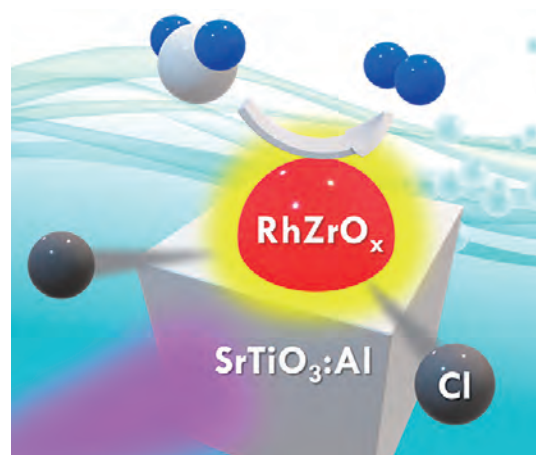


Figure 2. Illustration of RhZrO_x cocatalyst on $\text{SrTiO}_3:\text{Al}$ photocatalyst. RhZrO_x works as an active site for photocatalytic hydrogen evolution reaction. Active RhZrO_x cocatalyst is formed by the spontaneous Cl^- removal from preformed Rh–Cl–Zr–O solid during photocatalysis.

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MORANDINI, Andrea Università Ca' Foscari Venezia, Italy, 2 October 2019–3 February 2020

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 Living Radical Polymerization
Polymer Brush Hybrid Materials
Biointerface



Selected Publications

Hsu, S.-Y.; Kayama, Y.; Ohno, K.; Sakakibara, K.; Fukuda, T.; Tsujii, Y., Controlled Synthesis of Concentrated Polymer Brushes with Ultralarge Thickness by Surface-Initiated Atom Transfer Radical Polymerization under High Pressure, *Macromolecules*, **53**, 132-137 (2020).
Sakakibara, K.; Wakiuchi, A.; Murata, Y.; Tsujii, Y., Precise Synthesis of Double-armed Polymers with Fullerene C₆₀ at the Junction for Controlled Architecture, *Polym. Chem.*, **11**, 4417-4425 (2020).
Tadokoro, C.; Sato, K.; Nagamine, T.; Nakano, K.; Sasaki, S.; Sato, T.; Sakakibara, K.; Tsujii, Y., Concentrated Polymer Brush as Reciprocating Seal Material for Low Leakage and Low Friction, *Tribology Transactions*, **63**, 20-27 (2020).
Hsu, S.-Y.; Ohno, K.; Sakakibara, K.; Tsujii, Y., Convenient Synthesis of Very-Thick Concentrated Polymer Brushes by Atom Transfer Radical Polymerization in an Ionic Liquid, *Macromolecules*, **53**, 7936-7943 (2020).
Sakakibara, K.; Moriki, Y.; Tsujii, Y., Simultaneous Nanofibrillation and Compounding of Wood Pulp Fibers Using Polyols as Plasticizers: Fabricating High-performance Cellulose-nanofiber-reinforced Polyethylene Composites, *J. Fiber Sci. Technol.*, **76**, 23-31 (2020).

Elasto-hydrodynamic Lubrication on Well-defined, Epoxy-Resin-Based Monolith Containing Ionic Liquid

We have successfully realized an elasto-hydrodynamic lubrication (EHL) on a monolithic thin film of well-defined, bicontinuous three-dimensional networks of polymer framework and pore, which is prepared through polymerization-induced phase separation in the presence of a non-reactive porogen. In the EHL as one of hydrodynamic lubrication mechanisms, the friction and wear can be reduced by significant elastic deformation of the surface and hence effective formation of lubricant layer between the rubbing (base) materials (inhibiting the direct contact). **Figure 1** schematically illustrates the experimental setup: the monolith surface was sputter-coated by aluminium to enhance the reflectivity, and the probe-glass lens was modified with a 480-nm silicate layer on a reflective Cr one to precisely determine a small thickness. **Figure 2** shows the measured film thickness h_c of the lubricant (poly- α -olefin, viscosity = 110 cP at 25 °C) as a function of sliding velocity v . In an immersed condition, the h_c value decreased with decreasing v with a slope of 0.58 in this plot, which is almost consistent with the EHL theory. It is surprising that the EHL mechanism was kept even at a lubricant-layer thickness of ~ 10 nm, much smaller than the surface roughness of the probe lens. Another important point is that even in a so-called “starved” condition, similar lubrication was

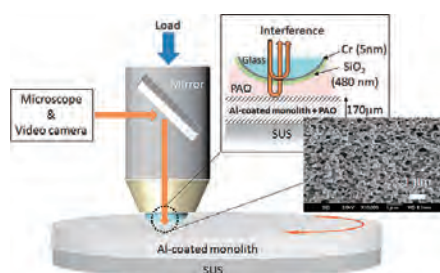


Figure 1. Schematic illustration of in-situ frictional/optical measurements in ball-on-disk setup.

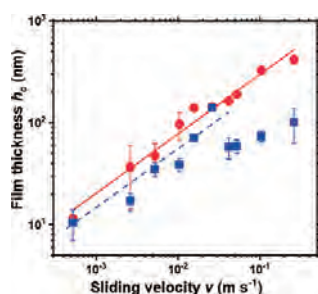


Figure 2. Double logarithmic plot of lubricant-film thickness h_c at a normal load of 1N against sliding velocity v in immersed (●) and starved (■) lubrication conditions using PAO as a lubricant.

achieved in a relatively low velocity. These tribological properties characteristic to the monolith materials is well understood from the viewpoint of the deformation of the polymer framework and the hydrodynamic effect of thus excluded lubricant. This monolith-coating system is expected to be applicable on various mechanical elements for their prolonged life and energy saving.

Controlling the Thermally Induced Phase Separation of Polymer/Ionic-Liquid Blended Films with Concentrated-Polymer-Brush-Decorated Hybrid Particles

The development of quasi-solid electrolytes for electrical devices operating at high voltages is important to address future energy storage requirements. Here, we report a new method to fabricate quasi-solid electrolytes through the thermally induced phase separation of a polymer/ionic-liquid (polymer/IL) blend. In a polymer/IL blend that exhibits lower critical solution temperature-type phase separation, we demonstrate that the addition of silica particles decorated with concentrated polymer brush (CPB-SiPs) can prevent the macroscopic phase separation after heating, resulting in a quasi-solid electrolyte with a continuous IL phase. This is due to the adsorption of CPB-SiPs onto the polymer/IL interface in the phase-separated structure. We also reveal a relationship between the molecular weight of the CPB and the phase-separated structure. Namely, a quasi-solid film with a bicontinuous phase-separated structure is formed only when polymers with an appropriate molecular weight are grafted on the CPB-SiPs (**Figure 3**). The resulting quasi-solid film exhibits a relatively high ionic conductivity, owing to the existence of a continuous ion-conductive phase solely consisting of IL. In addition, we fabricated a quasi-solid electrolyte with the blended film and successfully applied it to an electric double-layer capacitor operating at a high voltage, owing to the wider potential window of the IL employed herein.

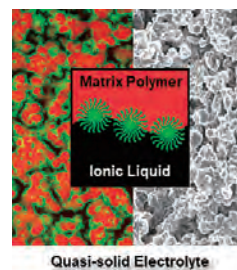


Figure 3. Confocal laser scanning microscopy and scanning electron microscopy images of polymer/ionic liquid blended films added with 10 wt% of polymer-brush-decorated nanoparticles. Red, black, and green correspond to the matrix polymer phase, ionic liquid phase, and nanoparticles, respectively.

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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.



KEYWORDS

Organic Synthesis

Polymer Properties

Polymer Synthesis

Curved π -Conjugated Molecules

Living Radical Polymerization

Selected Publications

Li, X.; Oghihara, T.; Abe, M.; Nakamura, Y.; Yamago, S., The Effect of Viscosity on the Diffusion and Termination Reaction of Organic Radical Pairs, *Chem. Eur. J.*, **25**, 9846-9850 (2019).

Lu, Y.; Yamago, S., Synthesis of Structurally Controlled, Highly Branched Polymethacrylates by Radical Polymerization Through the Design of a Monomer Having Hierarchical Reactivity, *Macromolecules*, **53**, 3209-3216 (2020).

Kayahara, E.; Nakano, M.; Sun, L.; Ishida, K.; Yamago, S., Syntheses of Tetrasubstituted [10]Cycloparaphenylenes by a Pd-catalyzed Coupling Reaction. Remarkable Effect of Strain on the Oxidative Addition and Reductive Elimination, *Chem. Asian J.*, **15**, 2451-2455 (2020).

Imamura, Y.; Fujita, T.; Kobayashi, Y.; Yamago, S., Tacticity, Molecular Weight, and Temporal Control by Lanthanide Triflate-Catalyzed Stereoselective Radical Polymerization of Acrylamides with an Organotellurium Chain Transfer Agent, *Polym. Chem.*, **11**, 7042-7049 (2020).

One-Step Synthesis of Dendritic Highly Branched Polystyrenes by Organotellurium-Mediated Copolymerization of Styrene and a Dienyl Telluride Monomer

By a one-step copolymerization of dienyly telluride (DT) and styrene (St) in the presence of organotellurium chain transfer agent (CTA) at thermal condition, dendritic highly branched polystyrenes (HB-PSts) were successfully synthesized. The molecular weight, branching density, and dendritic generation were easily controlled by the ratio of CTA, DT, and St with maintaining low dispersity ($D < 2.2$). The branching efficiency estimated by a deuterium-labeling experiment showed that DT quantitatively (>95%) served as the branching point. The end group fidelity was determined by the end group transformation to pyrene derivative and was proved to be high (ca. 90%). Intrinsic viscosity of the HB-PSt was significantly lower than that of linear polystyrenes and were easily tuned by the branching number and branching density. The method is compatible of various functional groups, and furthermore, chloro and acetoxy-substituted styrenes were also used as comonomer. A tadpole block copolymer was also synthesized by starting from linear PSt as a macroinitiator.

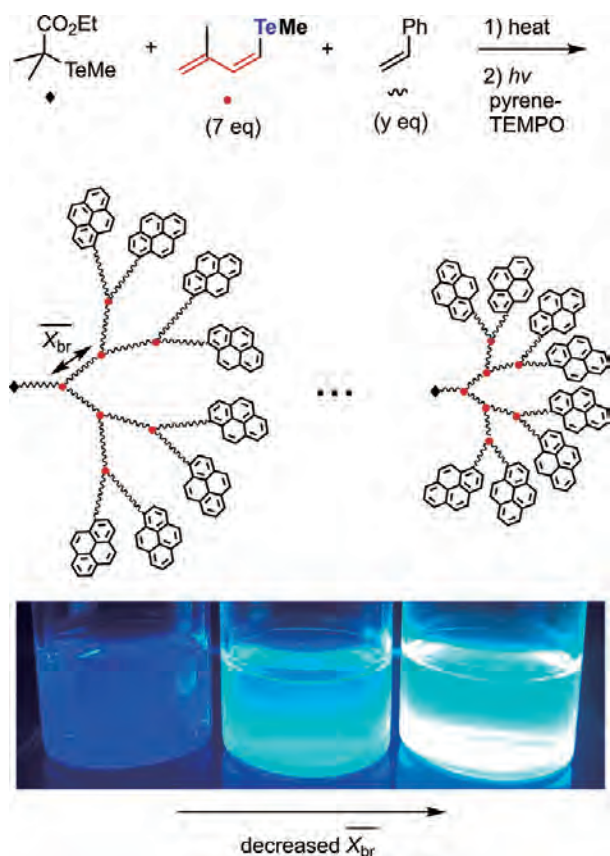


Figure 1. End group transformation of the highly branched polystyrene.

Syntheses of Tetrasubstituted [10]Cycloparaphenylenes by a Palladium-catalyzed Coupling Reaction. Remarkable Effect of Strain on the Oxidative Addition and Reductive Elimination

A small library of tetrasubstituted [10]cycloparaphenylene ([10]CPP) derivatives bearing alkyl, alkenyl, alkynyl and aryl substituents was constructed by a palladium-catalyzed cross-coupling reaction starting from tetratriflate [10]CPP, which was readily available in high yields on a >2 g scale. The CPP skeleton increases the reactivity of aryl triflate for oxidative addition to the palladium species, and the tetratriflate [10]CPP was found to be 10 times more reactive than its linear paraphenylene analogue, as determined by competition experiments. Theoretical calculations suggested that the accumulation of the small strain relief from each paraphenylene unit not involved in the reaction is responsible for the observed enhancement of reactivity.

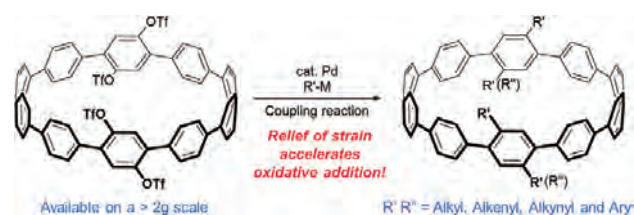


Figure 2. Synthesis of tetrasubstituted [10]cycloparaphenylene derivatives bearing alkyl, alkenyl, alkynyl and aryl substituents.

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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 spin-coherence time of the NV center is very long. The spin-coherence 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



Selected Publications

Herbschleb, E. D.; Kato, H.; Maruyama, Y.; Danjo, T.; Makino, T.; Yamasaki, S.; Ohki, I.; Hayashi, K.; Morishita, H.; Fujiwara, M.; Mizuochi, N., Ultra-long Coherence Times Amongst Room-temperature Solid-state Spins, *Nat. Commun.*, **10**, 3766 (2019).
Morishita, H.; Tashima, T.; Mima, D.; Kato, H.; Makino, T.; Yamasaki, S.; Fujiwara, M.; Mizuochi, N., Extension of the Coherence Time by Generating MW Dressed States in a Single NV Centre in Diamond, *Sci. Rep.*, **9**, 13318 (2019).
Tashima, T.; Morishita, H.; Mizuochi, N., Experimental Demonstration of Two-photon Magnetic Resonances in a Single-spin-system of a Solid, *Phys. Rev. A*, **100**, 023801 (2019).
Yamaguchi, T.; Matsuzaki, Y.; Saito, S.; Watanabe, H.; Mizuochi, N.; Ishi-Hayase, J., Bandwidth Analysis of AC Magnetic Field Sensing Based on Electronic Spin Double Resonance of Nitrogen-vacancy Centers in Diamond, *Jpn. J. Appl. Phys.*, **58**, 100901 (2019).

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 ^{12}C and ^{28}Si 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 single-crystal diamond realises remarkably long spin-coherence times. Single electron spins show the longest inhomogeneous spin-dephasing time ($T_2^* \approx 1.5$ 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 T_2 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.

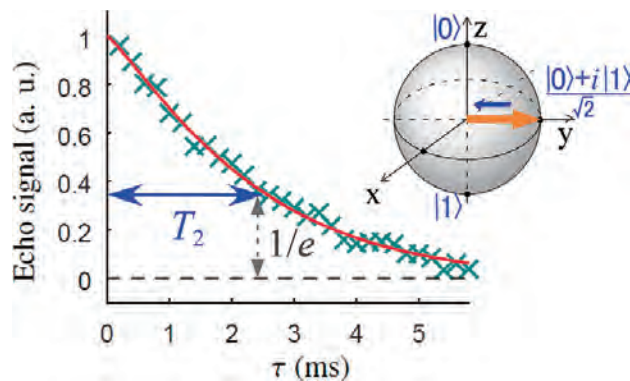


Figure 1. Echo signal of the single NV centre at room temperature. (Insert) Bloch sphere to show the coherence (superposition state).

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_{2p} 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.

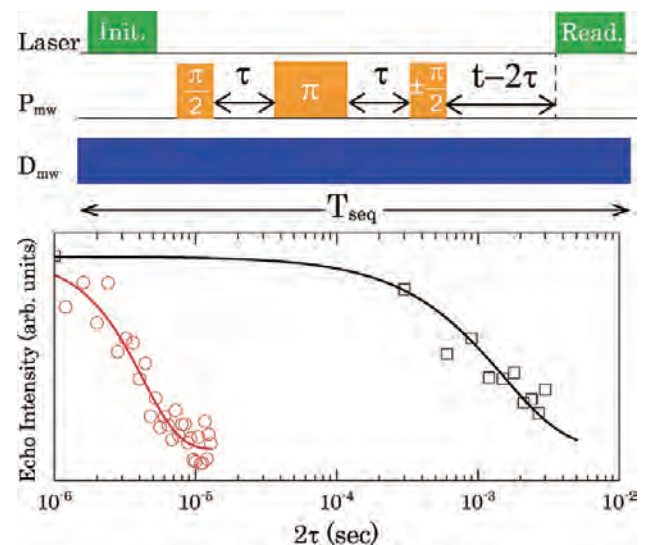


Figure 2. (Top) Pulse sequence to observe T_{2p} and T_2 with applying a phase cycle to the final $\pi/2$ pulse. (Bottom) Black and red plots show the results of T_{2p} and T_2 measurements, respectively. They are fitted by exponential decay curves described by black and red solid lines.

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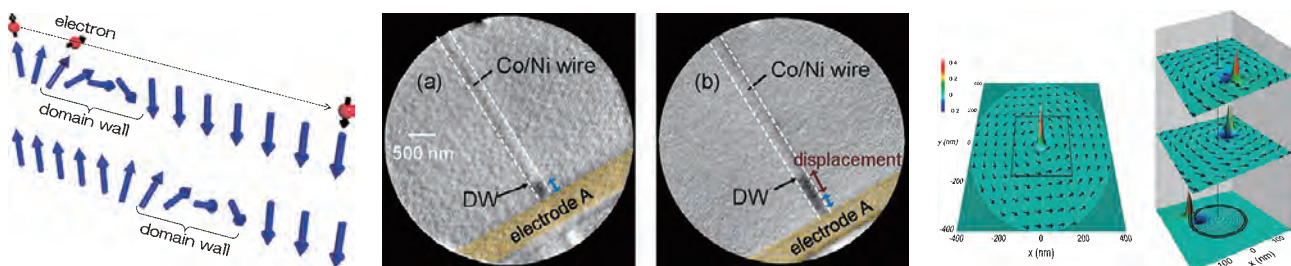
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Scope of Research

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



Selected Publications

Ando, F.; Miyasaka, Y.; Li, T.; Ishizuka, J.; Arakawa, T.; Shiota, Y.; Moriyama, T.; Yanase, Y.; Ono, T., Observation of Superconducting Diode Effect, *Nature*, **584**, 373-376 (2020).

Moriyama, T.; Hayashi, K.; Yamada, K.; Shima, M.; Ohya, Y.; Ono, T., Tailoring THz Antiferromagnetic Resonance of NiO by Cation Substitution, *Phys. Rev. Materials*, **4**, 074402 (2020).

Ishibashi, M.; Shiota, Y.; Li, T.; Funada, S.; Moriyama, T.; Ono, T., Switchable Giant Nonreciprocal Frequency Shift of Propagating Spin Waves in Synthetic Antiferromagnets, *Sci. Adv.*, **6**, eaaz6931 (2020).

Iwaki, H.; Kimata, M.; Ikebuchi, T.; Kobayashi, Y.; Oda, K.; Shiota, Y.; Ono, T.; Moriyama, T., Large Anomalous Hall Effect in L1₂-ordered Antiferromagnetic Mn₃Ir Thin Films, *Appl. Phys. Lett.*, **116**, 022408 (2020).

Okuno, T.; Kim, D.-H.; Oh, S.-H.; Kim, S.-K.; Hirata, Y.; Nishimura, T.; Ham, W.-S.; Futakawa, Y.; Yoshikawa, H.; Tsukamoto, A.; Tserkovnyak, Y.; Shiota, Y.; Moriyama, T.; Kim, K.-J.; Lee, K.-J.; Ono, T., Spin-transfer Torques for Domain Wall Motion in Antiferromagnetically Coupled Ferrimagnets, *Nat. Electron.*, **2**, 389-393 (2019).

Observation of Super Conducting Diode Effect

Nonlinear optical and electrical effects associated with a lack of spatial inversion symmetry allow direction-selective propagation and transport of quantum particles, such as photons and electrons. The most common example of such nonreciprocal phenomena is a semiconductor diode with a p–n junction, with a low resistance in one direction and a high resistance in the other. Although the diode effect forms the basis of numerous electronic components, such as rectifiers, alternating–direct-current converters and photodetectors, it introduces an inevitable energy loss due to the finite resistance. Therefore, a worthwhile goal is to realize a superconducting diode that has zero resistance in only one direction. Here we demonstrate a magnetically controllable superconducting diode in an artificial superlattice $[\text{Nb}/\text{V}/\text{Ta}]_n$ without a centre of inversion. The nonreciprocal resistance versus current curve at the superconducting-to-normal transition was clearly observed by a direct-current measurement, and the difference of the critical current is considered to be related to the magnetochiral anisotropy caused by breaking of the spatial-inversion and time-reversal symmetries. Owing to the nonreciprocal critical current, the $[\text{Nb}/\text{V}/\text{Ta}]_n$ superlattice exhibits zero resistance in only one direction. This superconducting diode effect enables phase-coherent and direction-selective charge transport, paving the way for the construction of non-dissipative electronic circuits.

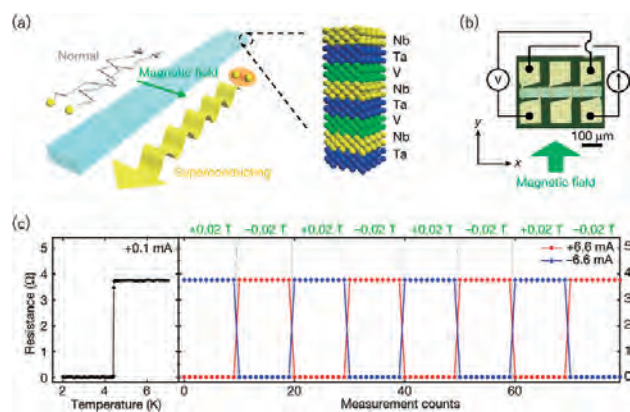


Figure 1. (a) Schematic images of the superconducting diode controlled by an external magnetic field and the artificial $[\text{Nb}/\text{V}/\text{Ta}]_n$ superlattice, in which the global inversion symmetry is broken along the direction of stacking. When the directions of the current, the magnetic field and inversion symmetry breaking are orthogonal to one other, the Cooper pairs can flow in only one direction. (b) Photomicrograph of the processed device and the measurement setup with the definitions of electric current and magnetic field. (c) Temperature dependence of the sheet resistance of the $[\text{Nb}(1.0 \text{ nm})/\text{V}(1.0 \text{ nm})/\text{Ta}(1.0 \text{ nm})]_{40}$ film and alternating switching between the superconducting and normal conducting states by changing the sign of the applied current or magnetic field at 4.2 K.

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). Antiferromagnets are considered one of the material candidates for the racetrack memory. However, experimental explorations of STT in antiferromagnets remain elusive because of experimental difficulty accessing some of the magnetic properties. In this work, we instead examined the effects of STT in a ferrimagnetic material (a GdFeCo alloy), a more experimentally accessible material, which mimics an antiferromagnetic property at a certain temperature, the so-called angular momentum compensation temperature T_A . We measured the DW velocity under the application of electric current at various temperatures (see Figure 2(a) for the experimental setup). We found that, as shown in Figure 2(b), the DW velocity changes its sign in the vicinity of T_A . By fitting the experimental data with the theoretical model, we quantitatively determined the two components of STT, *i.e.* the adiabatic and non-adiabatic torques. Our result show that the non-adiabatic STT in antiferromagnets is indeed quite large, suggesting that an energy-efficient DW racetrack memory may be possible with antiferromagnets.

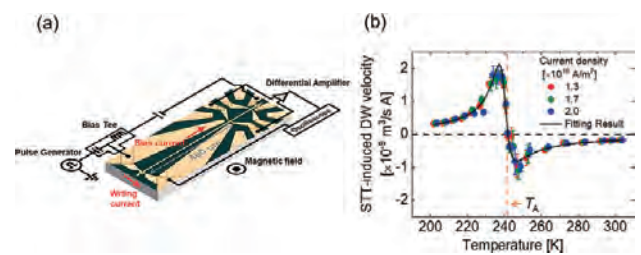


Figure 2. (a) Schematic illustration of the experimental setup. (b) The STT-induced DW velocity as a function of temperature. The dotted orange line represents the angular momentum compensation temperature T_A .

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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

Selected Publications

Arafiles, J. V. V.; Hirose, H.; Akishiba, M.; Tsuji, S.; Imanishi, M.; Futaki, S., Stimulating Macropinocytosis for Intracellular Nucleic Acid and Protein Delivery: A Combined Strategy with Membrane-Lytic Peptides to Facilitate Endosomal Escape, *Bioconjug. Chem.*, **31**, 547-553 (2020).
Masuda, T.; Hirose, H.; Baba, K.; Walrant, A.; Sagan, S.; Inagaki, N.; Fujimoto, T.; Futaki, S., An Artificial Amphiphilic Peptide Promotes Endocytic Uptake by Inducing Membrane Curvature, *Bioconjug. Chem.*, **31**, 1611-1615 (2020).
Ohtani, R.; Kawano, K.; Kinoshita, M.; Yanaka, S.; Watanabe, H.; Hirai, K.; Futaki, S.; Matsumori, N.; Uji-i, H.; Ohba, M.; Kato, K.; Hayami, S., Pseudo-Membrane Jackets: Two-Dimensional Coordination Polymers Achieving Visible Phase Separation in Cell Membrane, *Angew. Chem. Int. Ed.*, **59**, 17931-17937 (2020).
Shinoda, K.; Suda, A.; Otonari, K.; Futaki, S.; Imanishi, M., Programmable RNA Methylation and Demethylation Using PUF RNA Binding Proteins, *Chem. Commun.*, **56**, 1365-1368 (2020).
Kawano, K.; Yokoyama, F.; Kawamoto, J.; Ogawa, T.; Kurihara, T.; Futaki, S., Development of a Simple and Rapid Method for *In Situ* Vesicle Detection in Cultured Media, *J. Mol. Biol.*, **432**, 5876-5888 (2020).

Curvature-sensing Peptides to Distinguish Bacterial Extracellular Membrane Vesicles from Cells in Cultured Medium

Extracellular membrane vesicles (EMVs) are biogenic secretory lipidic vesicles that play significant roles in intercellular communication related to human diseases and bacterial pathogenesis. They are being investigated for their possible use in diagnosis, vaccines, and biotechnology. However, the existing methods suffer from a number of issues. High-speed centrifugation, a widely used method to collect EMVs, may cause structural artifacts. Immunostaining methods require several steps and thus the separation and detection of EMVs from the secretory cells is time-consuming. Furthermore, detection of EMVs using these methods requires specific and costly antibodies. To tackle these problems, development of a simple and rapid detection method for the EMVs in the cultured medium without separation from the secretory cells is a pressing task. In this study, we focused on the Gram-negative bacterium *Shewanella vesiculosa* HM13, which produces a large amount of EMVs including a cargo protein with high purity, as a model [C. Chen, *et al.*, *Front. Microbiol.*, **2020**, 10, 3001]. FAAV, a curvature-sensing peptide [K. Kawano, *et al.*, *Chem. Pharm. Bull.*, **2019**, 67, 1131], selectively binds to the EMVs even in the presence of the secretory cells in the complex cultured medium (Figure 1). FAAV can fully detect the EMVs within a few minutes, and the resistance of FAAV to proteases enables it to withstand prolonged use in the cultured medium. Fluorescence / Förster resonance energy transfer (FRET) was used to develop a method to detect changes in the amount of the EMVs with high sensitivity. Overall, our results indicate the potential applicability of FAAV for *in situ* EMV detection in cultured media.

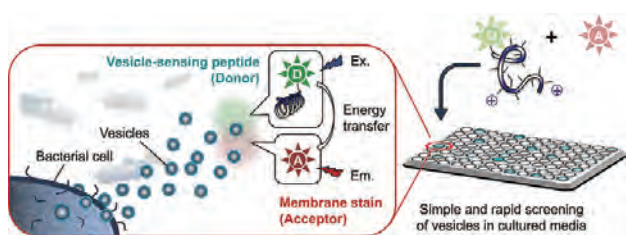


Figure 1. A method for *in situ* vesicle detection in cultured media.

Targeted RNA Methylation and Demethylation Using Artificial RNA Binding Proteins

*N*6-methyladenosine (^m6A) is the most abundant internal RNA modification in eukaryotic mRNA, regulating various aspects of mRNA metabolism, such as mRNA stability, localization, and translation, ultimately controlling gene expression. The levels of ^m6A methylation are controlled by ^m6A regulatory enzymes. METTL3 and METTL14 form a heterodimer and install the methyl group into *N*6-adenosine within the RRACH (R: A, G; H: A, C, U) sequences. FTO or ALKBH5 catalyses demethylation. Although sequencing analysis using Me-RIP-seq and down- or up-regulation of the ^m6A regulatory enzymes have revealed the importance of ^m6A in various biological phenomena, the function of individual ^m6A has not yet been revealed. New methods to control local RNA methylation are needed. Here fusion proteins of ^m6A regulatory enzymes, FTO demethylase and METTL14 methyltransferase, with a programmable RNA binding protein, PUF, were designed (Figure 2). Sequence-specific (de)methylation was demonstrated *in vitro* even in the presence of excess amount of non-specific RNA fragments derived from mammalian cells, strongly suggesting these chimeras could be used in transcriptome. This study provides a proof-of-principle that the strategy to fuse ^m6A-regulatory enzymes with the programmable RNA binding protein PUF is a promising way for site-specific control of RNA methylation, not only at the transcript level but also at the level of a single ^m6A site within a given transcript to clarify the function of individual RNA methylation.

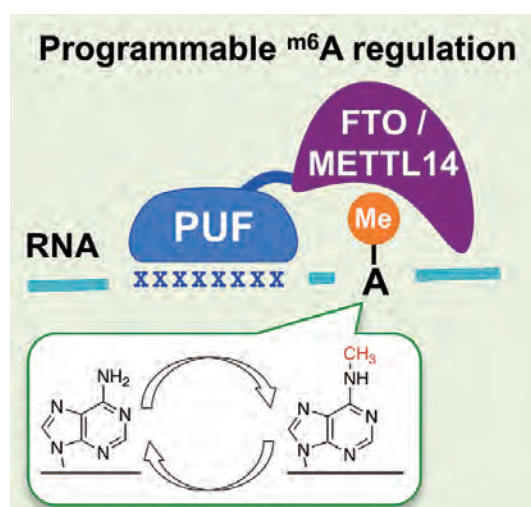


Figure 2. Targeted RNA methylation and demethylation using fusion proteins of RNA (de)methylases with programmable RNA binding protein, PUF.

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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



Selected Publications

Yasui, R.; Seto, Y.; Ito, S.; Kawada, K.; Itto-Nakama, K.; Mashiguchi, K.; Yamaguchi, S., Chemical Screening of Novel Strigolactone Agonists that Specifically Interact with DWARF14 Protein, *Bioorg. Med. Chem. Lett.*, **29**, 938-942 (2019).

Seto, Y.; Yasui, R.; Kameoka, H.; Tamiru, M.; Cao, M.; Terauchi, R.; Sakurada, A.; Hirano, R.; Kisugi, T.; Hanada, A.; Umehara, M.; Seo, E.; Akiyama, K.; Burke, J.; Takeda-Kamiya, N.; Li, W.; Hirano, Y.; Hakoshima, T.; Mashiguchi, K.; Noel, J. P.; Kyojuka, J.; Yamaguchi, S., Strigolactone Perception and Deactivation by a Hydrolase Receptor DWARF14, *Nat. Commun.*, **10**, [191-1]-[191-10] (2019).

Burger, M.; Mashiguchi, K.; Lee, H. J.; Nakano, M.; Takemoto, K.; Seto, Y.; Yamaguchi, S.; Chory, J., Structural Basis of Karrikin and Non-natural Strigolactone Perception in *Physcomitrella patens*, *Cell Rep.*, **26**, 855-865 (2019).

Mashiguchi, K.; Hisano, H.; Takeda-Kamiya, N.; Takebayashi, Y.; Ariizumi, T.; Gao, Y.; Ezura, H.; Sato, K.; Zhao, Y.; Hayashi, K.; Kasahara, H., *Agrobacterium tumefaciens* Enhances Biosynthesis of Two Distinct Auxins in the Formation of Crown Galls, *Plant Cell Physiol.*, **60**, 29-37 (2019).

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 (T_m) shift of AtD14, suggesting that SLs trigger the active state of D14 before their hydrolysis.

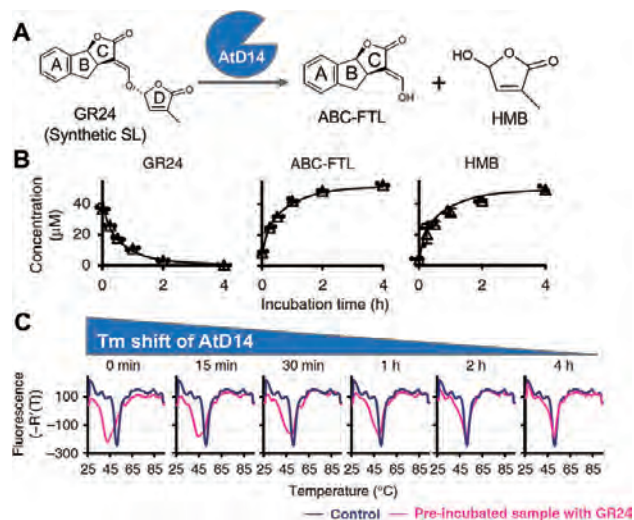


Figure 1. The time-course analyses of SL binding and hydrolysis by AtD14. (A) Hydrolysis reaction of SL (GR24) by AtD14. (B) Quantification of the hydrolysis reaction of GR24 (40 μ M) by AtD14. (C) The T_m shift of AtD14 incubated with GR24 (40 μ M) in DSF analysis. The maximum T_m shift was observed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

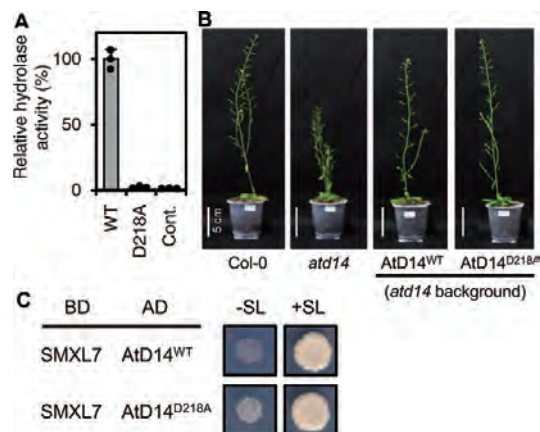


Figure 2. Functional analysis of the AtD14^{D218A} mutant. (A) The SL hydrolysis activities of maltose binding protein (MBP)-tagged wild-type of AtD14 protein (AtD14^{WT}) and the AtD14^{D218A} mutant. MBP was used in the control reaction. (B) The branching phenotype of Arabidopsis transgenic plants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

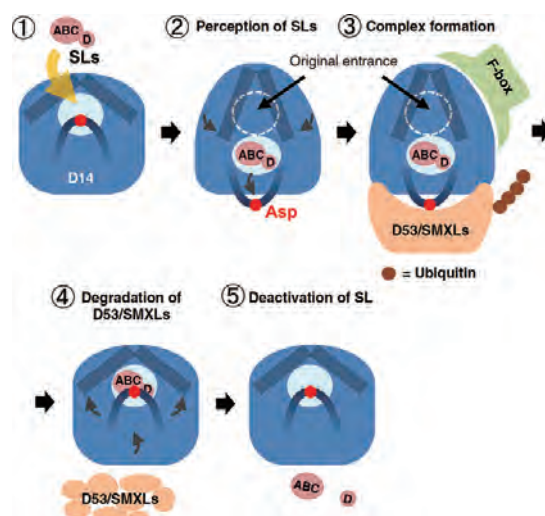


Figure 3. A proposed model of D14 in SL signaling. Bioactive SLs induce the conformational changes of D14, which triggers complex formation with the signaling partners. After the degradation of negative regulators of SL signaling (D53/SMXLs) and transmission of the SL signal, D14 reconstructs the catalytic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

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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) the transcriptional network for cytokinin responses, 3) COP9 signalosome modulating signal transduction in the nuclei, and 4) the endoreduplication cell cycle in cell differentiation.

KEYWORDS

Morphogenesis Signal Transduction
Phospholipid Signaling COP9 Signalosome
RNA



Selected Publications

Kato, M.; Tsuge, T.; Maeshima, M.; Aoyama, T., *Arabidopsis* PCaP2 Modulates the Phosphatidylinositol 4,5-bisphosphate Signal on the Plasma Membrane and Attenuates Root Hair Elongation, *Plant J.*, **99**, 610-625 (2019).
Lin, Q.; Ohashi, Y.; Kato, M.; Tsuge, T.; Gu, H.; Qu, L.-J.; Aoyama, T., GLABRA2 Directly Suppresses Basic Helix-loop-helix Transcription Factor Genes with Diverse Functions in Root Hair Development, *Plant Cell*, **27**, 2894-2906 (2015).
Wada, Y.; Kusano, H.; Tsuge, T.; Aoyama, T., Phosphatidylinositol Phosphate 5-kinase Genes Respond to Phosphate Deficiency for Root Hair Elongation in *Arabidopsis thaliana*, *Plant J.*, **81**, 426-437 (2015).
Hayashi, K.; Nakamura, S.; Fukunaga, S.; Nishimura, T.; Jenness, M. K.; Murphy, A. S.; Motose, H.; Nozaki, H.; Furutani, M.; Aoyama, T., Auxin Transport Sites are Visualized in Planta Using Fluorescent Auxin Analogs, *Proc. Natl. Acad. Sci. USA*, **111**, 11557-11562 (2014).
Kato, M.; Aoyama, T.; Maeshima, M., The Ca²⁺-binding Protein PCaP2 Located on the Plasma Membrane is Involved in Root Hair Development as a Possible Signal Transducer, *Plant J.*, **74**, 690-700 (2013).

Functions of Phosphatidylinositol 4-Phosphate 5-Kinases and Its Product Phosphatidylinositol 4,5-bisphosphate in Plant Cell Morphogenesis

Plants show us a lot of interesting shapes, which are determined by not only the architecture of cell propagation but also the morphology of each cell. In addition, each single cell often exhibits an elaborate shape serving its physiological role (Figure 1). Since plant cell morphogenesis, a process always accompanied with cell wall expansion, is irreversible, it should be progressed in a strictly regulated manner. How can plants regulate cell morphogenesis appropriately? To elucidate molecular mechanisms regulating plant cell morphogenesis, we are studying on phosphoinositide signaling, mainly that of Phosphatidylinositol 4,5-bisphosphate [PIP(4,5)P₂].

PIP(4,5)P₂, a minor phospholipid component of eukaryotic membranes, is involved in the regulation of various intracellular events. PIP(4,5)P₂ physically interacts with regulatory proteins for actin cytoskeletal organization and membrane trafficking on the plasma membrane. In addition, its signaling pathways are frequently connected to those of small GTPases belonging to the Rho and Arf families in their upstream and downstream cascades. PI(4,5)P₂ is expected to play a regulatory role in the polarized expansion of plant cells. Indeed, PI(4,5)P₂ exhibits polar localization patterns in various types of cells, including root hairs, pollen tubes, stomatal guard cells and root epidermal cells (Figure 2). We are focusing on functions of PI(4,5)P₂ and its producing enzymes, Phosphatidylinositol 4-phosphate 5-kinases (PIP5Ks), in cell morphogenesis.

The model plant *Arabidopsis thaliana* encodes two type-A and nine type-B PIP5Ks (Figure 3). Of these, four clades of type-B PIP5Ks, I, II, III and IV, containing *Arabidopsis* PIP5K1-3, PIP5K4-6, PIP5K7-8, and PIP5K9, respectively, are conserved in angiosperms. Type-B PIP5Ks are thought to redundantly play pivotal roles in various processes of plant cells while type-A PIP5Ks are thought to function only in pollens. To elucidate functions of type-B PIP5Ks in cell morphogenesis, we performed genetic analysis using multiple mutants of their genes. As the result, we identified triple mutants with phenotypes that have not seen in single or double mutants of type-B PIP5K genes so far, including those of no root hairs, no pollen tubes, and hypersensitivity to high osmolality. Interestingly, the mutant genes in each triple mutant are not always limited to genes in a single clade, suggesting that type-B PIP5K genes have been evolutionally differentiated in a complicated manner.

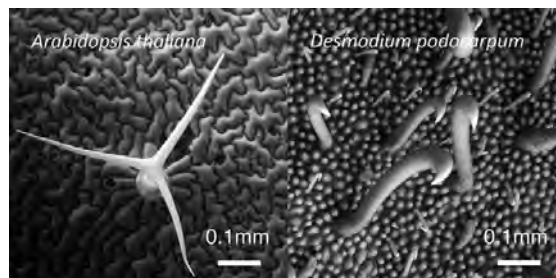


Figure 1. The leaf surface of *Arabidopsis thaliana* (thale cress) (left) and the seed pod surface of *Desmodium podocarpum* (Japanese bush clover) (right) were observed by scanning electron microscopy. (left) The leaf epidermis of *Arabidopsis thaliana* is covered with a branched spine-like structure called as trichome. Cells making a jigsaw puzzle-like pattern are leaf epidermal cells. (right) The seedpod epidermis of *Desmodium podocarpum* is covered with cells of a bead-like shape and a hook-like shape. The hook-like cells are also trichomes.

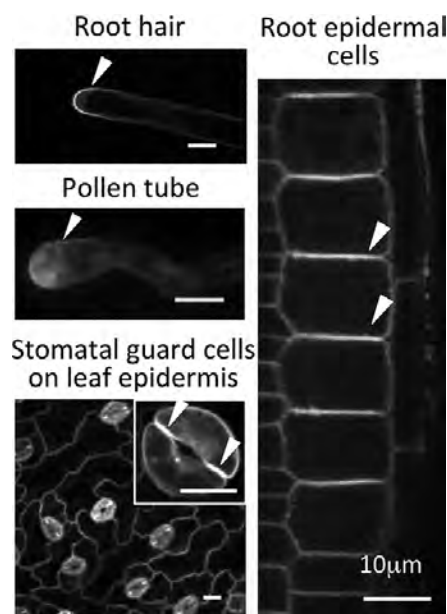


Figure 2. Subcellular localization patterns of the PI(4,5)P₂ marker, UBQ10 promoter-driven fluorescence protein fusion of 2xPH^{PLC8}, were observed in a root hair, a pollen tube, leaf epidermal cells, and root epidermal cells by confocal laser-scanning microscopy. Arrowheads indicate loci where the PI(4,5)P₂ marker are preferentially localized.

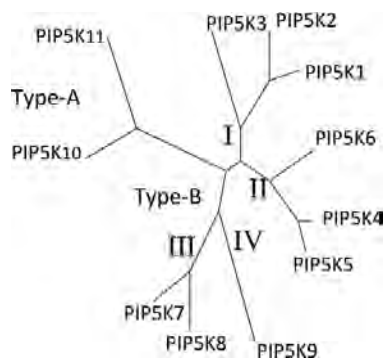


Figure 3. Phylogenetic tree of *Arabidopsis thaliana* type-A and type-B PIP5Ks are shown. Clades conserved in angiosperms are labeled as I, II, III, and IV.

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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, including future concepts in drug discovery and use of small molecules for immunotherapy.

KEYWORDS

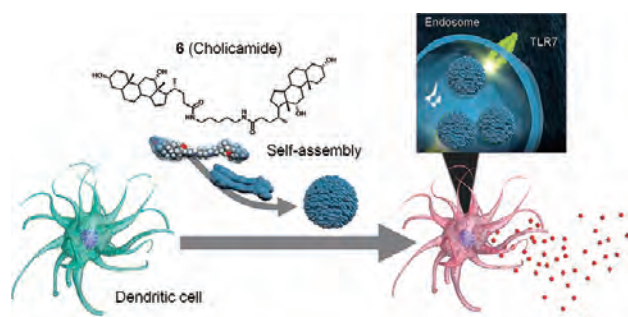
Chemical Biology Small Molecules Chemical Library
Chemical Genetics Immunology

Selected Publications

Jin, S.; Vu, H. V.; Hioki, K.; Noda, N.; Yoshida, H.; Shimane, T.; Ishizuka, S.; Takashima, I.; Mizuhata, Y.; Pe, K. B.; Ogawa, T.; Nishimura, N.; Packwood, D.; Tokitoh, N.; Kurata, H.; Yamasaki, S.; Ishii, K. J.; Uesugi, M., Discovery of Self-Assembling Small Molecules as Vaccine Adjuvants, *Angew. Chem. Int. Ed.*, **60**(2), 961-969 (2021).
Punzalan, L. L.; Jiang, L.; Mao, D.; Mahapatra, A. D.; Sato, S.; Takemoto, Y.; Tsujimura, M.; Kusamori, K.; Nishikawa, M.; Zhou, L.; Uesugi, M., Chemoproteomic Profiling of a Pharmacophore-Focused Chemical Library, *Cell Chem. Biol.*, **27**, 708-718 (2020).
Zhang, X.; Jiang, L.; Huang, K.; Fang, C.; Li, J.; Yang, J.; Li, H.; Ruan, X.; Wang, P.; Mo, M.; Wu, O.; Xu, Y.; Peng, C.; Uesugi, M.; Ye, D.; Yu, F.-X.; Zhou, L., Site-Selective Phosphoglycerate Mutase 1 Acetylation by a Small Molecule, *ACS Chem. Biol.*, **15**(3), 632-639 (2020).
Takemoto, Y.; Mao, D.; Punzalan, L. L.; Götze, S.; Sato, S.; Uesugi, M., Discovery of a Small-Molecule-Dependent Photolytic Peptide, *J. Am. Chem. Soc.*, **142**(3), 1142-1146 (2020).

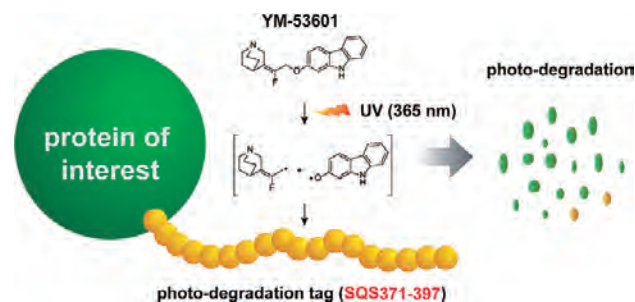
Discovery of Self-Assembling Small Molecules as Vaccine Adjuvants

Immune potentiators, termed adjuvants, trigger early innate immune responses to ensure the generation of robust and long-lasting adaptive immune responses of vaccines. Presented here is a study that takes advantage of a self-assembling small-molecule library for the development of a novel vaccine adjuvant. Cell-based screening of the library and subsequent structural optimization led to the discovery of a simple, chemically tractable deoxycholate derivative (molecule 6, also named cholicamide) whose well-defined nanoassembly potentially elicits innate immune responses in macrophages and dendritic cells. Functional and mechanistic analyses indicate that the virus-like assembly enters the cells and stimulates the innate immune response through Toll-like receptor 7 (TLR7), an endosomal TLR that detects single-stranded viral RNA. As an influenza vaccine adjuvant in mice, molecule 6 was as potent as Alum, a clinically used adjuvant. The studies described here pave the way for a new approach to discovering and designing self-assembling small-molecule adjuvants against pathogens, including emerging viruses.



Discovery of a Small-Molecule-Dependent Photolytic Peptide

We accidentally found that YM-53601, a known small-molecule inhibitor of squalene synthase (SQS), selectively depletes SQS from mammalian cells upon UV irradiation. Further analyses indicated that the photodepletion of SQS requires its short peptide segment located at the COOH terminus. Remarkably, when the 27 amino acid peptide was fused to green fluorescent protein or unrelated proteins at either the NH₂ or COOH terminus, such fusion proteins were selectively depleted when the cells were treated with both YM-53601 and UV exposure. Product analysis and electron spin resonance experiments suggested that the UV irradiation promotes homolytic C-O bond cleavage of the aryl ether group in YM-53601. It is likely that the radical species generated from UV-activated YM-53601 abstract hydrogen atoms from the SQS peptide, leading to the photolysis of the entire protein. The pair of the SQS peptide and YM-53601 discovered in the present study paves the way for the design of a new small-molecule-controlled optogenetic tool.



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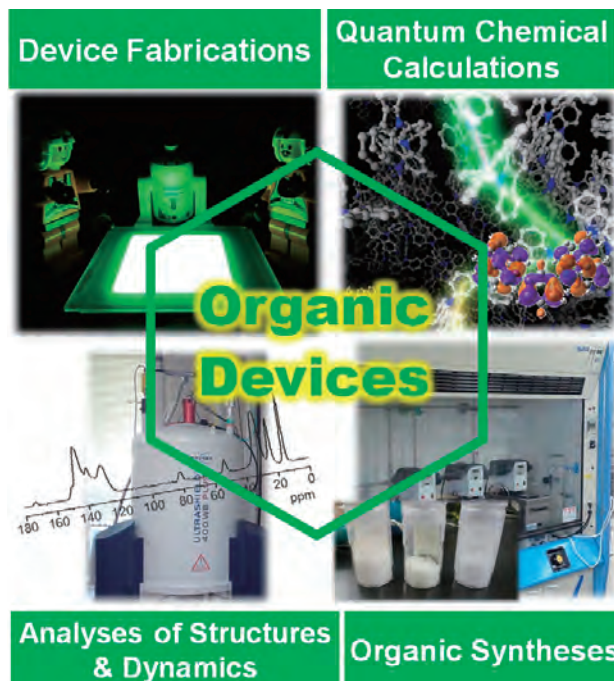
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SATO, Hiroki (UG)

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



Selected Publications

- Kusakabe, Y.; Wada, Y.; Nakagawa, H.; Shizu, K.; Kaji, H., Conformation Control of Iminodibenzyl-Based Thermally Activated Delayed Fluorescence Material by Tilted Face-to-Face Alignment with Optimal Distance (tFFO) Design, *Front. Chem.*, **8**, [530-1]-[530-9] (2020).
- Wada, Y.; Nakagawa, H.; Matsumoto, S.; Wakisaka, Y.; Kaji, H., Organic Light Emitters Exhibiting Very Fast Reverse Intersystem Crossing, *Nat. Photon.*, **14**, 643-649 (2020).
- Shizu, K.; Adachi, C.; Kaji, H., Visual Understanding of Vibronic Coupling and Quantitative Rate Expression for Singlet Fission in Molecular Aggregates, *Bull. Chem. Soc. Jpn.*, **93**, 1305-1313 (2020).
- Shizu, K.; Adachi, C.; Kaji, H., Effect of Vibronic Coupling on Correlated Triplet Pair Formation in the Singlet Fission Process of Linked Tetracene Dimers, *J. Phys. Chem. A*, **124**, 3641-3651 (2020).
- Shizu, K.; Adachi, C.; Kaji, H., Correlated Triplet Pair Formation Activated by Geometry Relaxation in Directly Linked Tetracene Dimer (5,5-Bitetracene), *ACS omega*, **6**, 2638-2643 (2021).

Thermally Activated Delayed Fluorescent Materials Showing Very Fast Reverse Intersystem Crossing

We report a robust molecular design, named “tilted Face-to-Face alignment with Optimal distance (tFFO),” for thermally activated delayed fluorescence materials showing very fast reverse intersystem crossing (RISC). tFFO design simultaneously realizes near-degenerate ^1CT , ^3CT and ^3LE states (where ^1CT and ^3CT denote singlet and triplet charge transfer states, respectively and ^3LE denotes triplet locally excited state) and notable spin-orbit coupling between them by controlling the through-space distance between the donor and acceptor segments in a molecule with tilted intersegment angles. Based on the concept, the first example molecule, TpAT-tFFO, realized very fast RISC with a rate constant of $1.2 \times 10^7 \text{ s}^{-1}$. In its application to organic light-emitting diodes, TpAT-tFFO exhibited high performance even at very high brightness owing to the ultrafast RISC. Our tFFO strategy can be versatily expanded to various types, numbers, and combinations of segments.

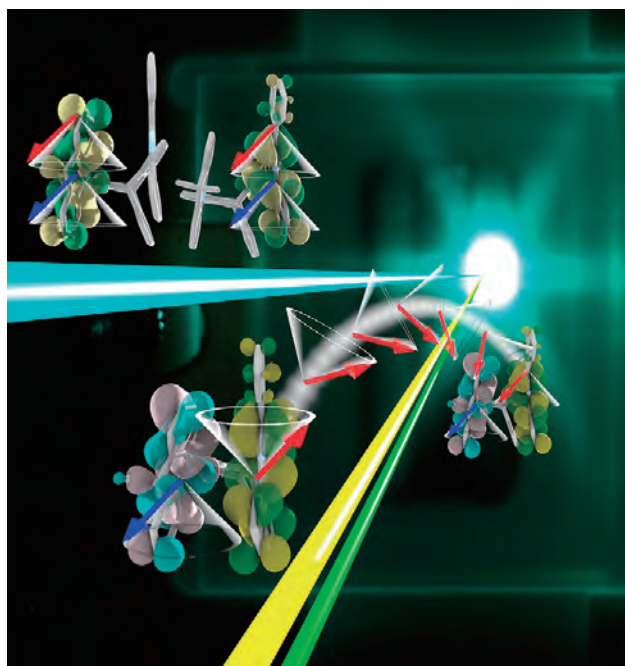


Figure 1. A thermally activated delayed fluorescence molecule showing very fast reverse intersystem crossing.

Singlet Fission Materials for Triplet Sensitizers in Organic Optoelectronics

Singlet fission (SF) or singlet-exciton fission is a multi-excitonic process that splits one singlet exciton into two triplet excitons. SF molecules are potential candidates for triplet sensitizers in organic light-emitting diodes. We develop a simple method for quantitatively predicting the SF efficiency on the basis of quantum chemical calculation and the Fermi golden rule. We apply this method to various SF molecules. Calculated SF rates are quantitatively consistent with experimental results, suggesting the validity of our method. Towards more realistic model, we combine the above approach with quantum mechanics/molecular mechanics (QM/MM) method to consider effects of environment on SF mechanism in molecular aggregates. Using the combined method, we quantitatively reproduce the SF rate in crystalline tetracene.

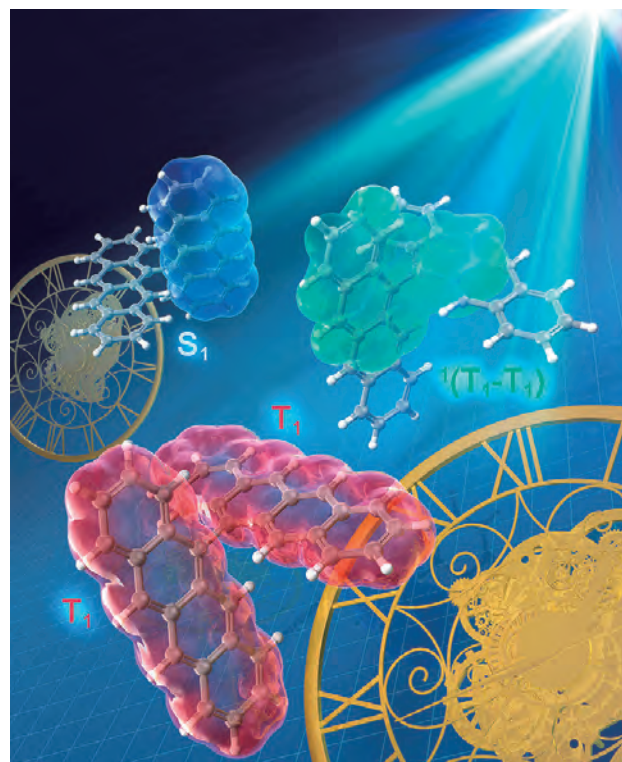


Figure 2. Theoretical design of singlet fission molecules.

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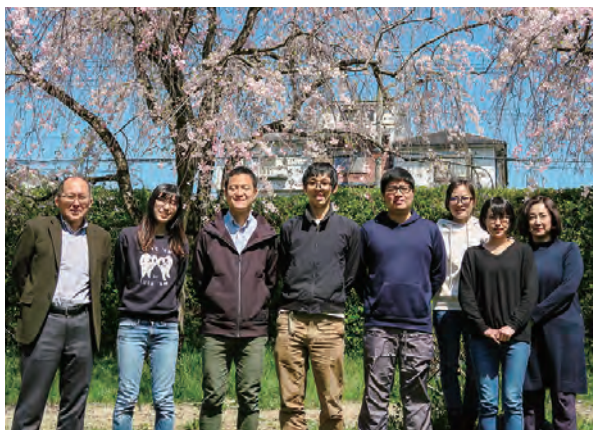
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Guest Res Assoc

MAHBOOB, Alam Banaras Hindu University, India, 22 January–20 March

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 Analytical Chemistry Trace Elements
Stable Isotopes Metal Ion Recognition

Selected Publications

Tsujsisaka, M.; Takano, S.; Murayama, M.; Sohrin, Y., Precise Analysis of the Concentrations and Isotopic Compositions of Molybdenum and Tungsten in Geochemical Reference Materials, *Anal. Chim. Acta*, **1091**, 146-159 (2019).
Takano, S.; Liao, W.-H.; Tian, H.-A.; Huang, K.-F.; Ho, T.-Y.; Sohrin, Y., Sources of Particulate Ni and Cu in the Water Column of the Northern South China Sea: Evidence from Elemental and Isotope Ratios in Aerosols and Sinking Particles, *Mar. Chem.*, **219**, 103751 (2020).
Liao, W.-H.; Takano, S.; Yang, S.-C.; Huang, K.-F.; Sohrin, Y.; Ho, T.-Y., Zn Isotope Composition in the Water Column of the Northwestern Pacific Ocean: The Importance of External Sources, *Global Biogeochem. Cy.*, **34**, e2019GB006379 (2020).
Fujiwara, Y.; Tsujisaka, M.; Takano, S.; Sohrin, Y., Determination of the Tungsten Isotope Composition in Seawater: The First Vertical Profile from the Western North Pacific Ocean, *Chem. Geol.*, **555**, 119835 (2020).
Nakaguchi, Y.; Ikeda, Y.; Sakamoto, A.; Zheng, L.; Minami, T.; Sohrin, Y., Distribution and Stoichiometry of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in the East China Sea, *Journal of Oceanography*, doi: 10.1007/s10872-020-00577-z (2020).

Sources of Particulate Ni and Cu in the Water Column of the Northern South China Sea

We present isotope ratios of Ni ($\delta^{60}\text{Ni}$) and Cu ($\delta^{65}\text{Cu}$) in sinking particles, aerosols, and seawater collected from the northern South China Sea. In aerosols, $\delta^{60}\text{Ni}$ values are in the range +0.05‰ to +0.56‰, and $\delta^{65}\text{Cu}$ values are in the range -0.33‰ to +0.83‰. The isotope ratios are different from those of lithogenic materials, indicating that the aerosols are anthropogenic in origin. In sinking particles collected at depths of 2,000 and 3,500 m, $\delta^{60}\text{Ni}$ values are in the range +0.01‰ to +0.54‰ at 2,000 m and -0.18‰ to +0.54‰ at 3,500 m, and the values exhibit a similar temporal variation pattern between 2,000 and 3,500 m. Based on the significant correlation between $\delta^{60}\text{Ni}$ and the ratio of P/Ni or organic-C/Ni, we hypothesize that the main sources of Ni in the sinking particles originate from both resuspended marine sediments off southwest Taiwan, and biogenic organic particles. The $\delta^{60}\text{Ni}$ in biogenic particles is estimated to be +0.6‰ to +1.0‰, which is 0.3–0.7‰ lighter than that of dissolved Ni in seawater. The isotope ratios of Cu in sinking particles are fairly constant (+0.13‰ to +0.36‰), and the range is between those of marine sediments and labile fractions of marine particles. Thus, Cu in sinking particles is likely to be from marine sediments and biogenic organic particles. Compared with Ni, the correlation between Cu and P or organic-C is weaker, suggesting that the Cu/P and Cu/organic-C ratios are not constant in organic matter or there are additional sources of particulate Cu, such as Fe-Mn oxides and anthropogenic aerosols.



Figure 1. Collaboration with Dr. Ho's group, Academia Sinica during the visit of S.T. supported by ICR-iJURC Short-term Exchange Program.

Determination of the Tungsten Isotope Composition in Seawater

The stable isotope ratio of W is a new tracer in oceanographic studies and a new proxy in paleoceanographic studies; however, precise data for modern seawater have not been reported to date. Because the concentration of W in seawater is as low as 49 pmol kg^{-1} , an ~3000-fold pre-concentration is necessary prior to measurement by multi-collector inductivity coupled plasma mass spectrometry (MC-ICP-MS). For the pre-concentration, we investigated solid-phase extraction using chelating resins, namely, NOBIAS Chelate-PA1 with ethylenediaminetriacetic acid groups and TSK-8HQ with 8-hydroxyquinoline groups. We report that TSK-8HQ is useful because the effects of the seawater matrix are minor thermodynamically and kinetically. We present a novel method for analysis of the concentrations and isotope ratios of W and Mo in seawater, consisting of solid phase extraction, chromatographic separation using anion exchange resin AG1 X8, and measurement by MC-ICP-MS. Both W and Mo are quantitatively recovered by this method, which was applied to seawater samples collected from the North Pacific Ocean. The measured concentration of W and the concentration and isotope ratio of Mo are consistent with those in the literature. The isotope ratio of W is found to be uniform throughout the water column in the western North Pacific Ocean; $\delta^{186/184}\text{W}$ is $0.55 \pm 0.12\%$ (ave $\pm 2\text{sd}$, $n = 7$) using NIST SRM 3163 as a reference for W. On the basis of this data, we determined that the isotopic difference in $\delta^{186/184}\text{W}$ is ~0.49‰ between seawater and oxic sediments in the modern ocean. This value accords with the reported experimental data for the isotope fractionation of W during adsorption on Mn and Fe (oxyhydr)oxides, suggesting the validity of our data.

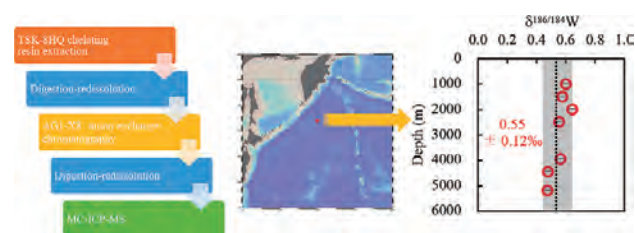


Figure 2. Schematic of the study.

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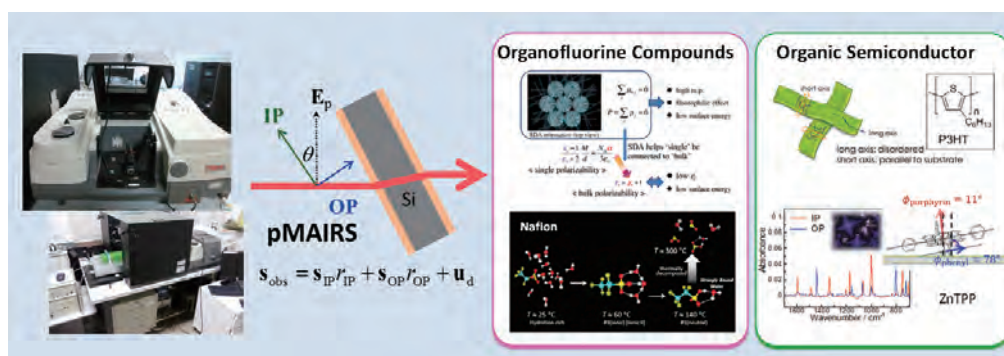
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Scope of Research

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



Selected Publications

Shioya, N.; Eda, K.; Shimoaka, T.; Hasegawa, T., Hidden Thin-Film Phase of Dinaphthothienothiophene Revealed by High-Resolution X-Ray Diffraction, *Appl. Phys. Express*, **13**, 095505 (2020).

Fukumi, A.; Shimoaka, T.; Shioya, N.; Nagai, N.; Hasegawa, T., Infrared Active Surface Modes Found in Thin Films of Perfluoroalkanes Reveal the Dipole–Dipole Interaction and Surface Morphology, *J. Chem. Phys.*, **153**, 044703 (2020).

Hasegawa, T.; Shioya, N., MAIRS: Innovation of Molecular Orientation Analysis in a Thin Film, *Bull. Chem. Soc. Jpn.*, **93**, 1127-1138 (2020).

Shioya, N.; Fujiwara, R.; Tomita, K.; Shimoaka, T.; Hasegawa, T., Simultaneous Analysis of Molecular Orientation and Quantity Change of Constituents in a Thin Film Using pMAIRS, *J. Phys. Chem. A*, **124**, 2714-2720 (2020).

MAIRS: Innovation of Molecular Orientation Analysis in a Thin Film

Multiple-angle incidence resolution spectrometry (MAIRS), originally developed in our group, is a unique spectroscopic technique for analyzing the structure of molecular aggregates in a thin film, which requires only the refractive index of the film for attaining an analytical accuracy of three significant digits (Figure 1). Since MAIRS is robust to the surface roughness of the film, rough films prepared by using the spin-coating, bar-coating, or drop-casting techniques can be analyzed with a good reproducibility. MAIRS makes the best use of a Fourier transform infrared (FT-IR) spectrometry, which enables us to discuss molecular conformation, packing, polymorphs etc. as well as the molecular orientation. At the moment, MAIRS has two options, pMAIRS and MAIRS2. pMAIRS has already been established and the application is spreading. MAIRS2 is the newest technology, which frees us from FT-IR specific problems, that is to say, interference of water-vapor peaks and of optical fringes.

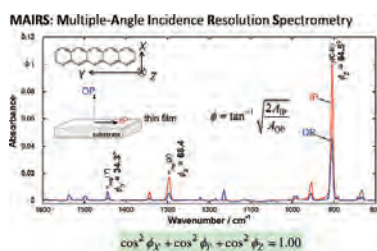


Figure 1. A pMAIRS spectrum of a pentacene film deposited on a Si substrate.

Infrared Active Surface Modes Found in Thin Films of Perfluoroalkanes Reveal the Dipole–Dipole Interaction and Surface Morphology

Infrared (IR) spectra of an organic thin film are mostly understood by considering the normal modes of a single molecule, if the dipole–dipole (D–D) interaction is ignorable in the film. When the molecules have a chemical group having a large permanent dipole moment such as the C=O and C–F groups, the D–D interaction induces vibrational couplings across the molecules, which produces an extra band as a surface phonon or polariton band because of the small thickness. Since the dipole moment of an organic compound is much less than that of an inorganic ionic crystal, we have a problem that the extra band looks like a normal-mode band, which are difficult to be discriminated from each other. In fact, this visual similarity sometimes leads us to a wrong direction in chemical discussion because the direction of the transition moment of the extra band is

totally different from those of the normal modes. We reveal useful selection rules for discussing IR spectra of a thin film without performing the permittivity analysis. The apparent change in the spectral shape on decrease in the thickness of the sample (Figure 2) can be correlated with the morphological change in the film surface. This analytical technique has effectively been applied for studying the chemical properties of perfluoroalkanes as a chemical demonstration, which readily supports the stratified dipole-array theory for perfluoroalkyl compounds.

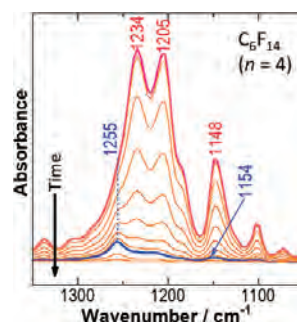


Figure 2. Time-dependent IR ATR spectra of C₆F₁₄ deposited on Ge during the evaporation process at ambient temperature.

Hidden Thin-Film Phase of Dinaphthothienothiophene Revealed by High-Resolution X-Ray Diffraction

Dinaphthothienothiophene (DNNT) has attracted considerable attention as a next-generation material for organic thin-film transistors, replacing the conventional basic material of pentacene. Although the performance of DNNT devices is higher than that of pentacene, and has been reported numerously, a comprehensive understanding of thin-film growth is lacking. In fact, thin-film structures have long been believed to be identical to single-crystal structures. In the present study, the thickness-dependent structural evolution is revealed by means of high-resolution X-ray diffraction. This technique apparently discriminates the thin-film structure from the conventionally known bulk structure (Figure 3). Thus, we have revealed the thin-film phase of DNNT for the first time.

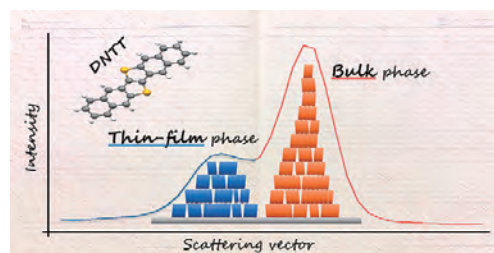


Figure 3. High-resolution X-ray diffraction measurements show two distinct peaks, which are newly assigned due to the thin-film and bulk phases.

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



Selected Publications

Chen, C.; Kawamoto, J.; Kawai, S.; Tame, A.; Kato, C.; Imai, T.; Kurihara, T., Isolation of a Novel Bacterial Strain Capable of Producing Abundant Extracellular Membrane Vesicles Carrying a Single Major Cargo Protein and Analysis of Its Transport Mechanism, *Front. Microbiol.*, **10**, 3001 (2020).

Ogawa, T.; Hirose, K.; Yustina, Y.; Kawamoto, J.; Kurihara, T., Bioconversion from Docosahexaenoic Acid to Eicosapentaenoic Acid in the Marine Bacterium *Shewanella livingstonensis* Ac10, *Front. Microbiol.*, **11**, 1104 (2020).

Kamasaka, K.; Kawamoto, J.; Chen, C.; Yokoyama, F.; Imai, T.; Ogawa, T.; Kurihara, T., Genetic Characterization and Functional Implications of the Gene Cluster for Selective Protein Transport to Extracellular Membrane Vesicles of *Shewanella vesiculosa* HM13, *Biochem. Biophys. Res. Commun.*, **526**, 525-531 (2020).

Yustina, Y.; Ogawa, T.; Kawamoto, J.; Kurihara, T., Role of Acyl-CoA Dehydrogenases from *Shewanella livingstonensis* Ac10 in Docosahexaenoic Acid Conversion, *Biochem. Biophys. Res. Commun.*, **528**, 453-458 (2020).

Toyotake, Y.; Nishiyama, M.; Yokoyama, F.; Ogawa, T.; Kawamoto, J.; Kurihara, T., A Novel Lysophosphatidic Acid Acyltransferase of *Escherichia coli* Produces Membrane Phospholipids with a *cis*-Vaccenoyl Group and is Related to Flagellar Formation, *Biomolecules*, **10**, 745 (2020).

Genetic Characterization of the Gene Cluster for Selective Cargo Transportation to Extracellular Membrane Vesicles of a Hyper-vesiculating Bacterium, *Shewanella vesiculosa* HM13

Bacteria release spherical nanoparticles enclosed by lipid membranes called extracellular membrane vesicles (EMVs), which selectively deliver various cellular components, such as DNA, lipids, lipopolysaccharides, and proteins, to their extracellular milieu. EMVs are involved in microbial interactions and survival in the hostile environment. Besides, EMVs have attracted the attention of biotechnological industries for their potential use as a vaccine, a carrier of drugs, and a platform for recombinant protein production.

Shewanella vesiculosa HM13, a Gram-negative bacterium isolated from fish intestine, produces a large amount of EMVs carrying an S-layer-like protein, P49, as a single major cargo of the EMVs. Secretion of P49 with high purity could be useful for secretory production of foreign protein. Whole genome sequencing of this strain has revealed that the gene coding for P49 is present in a gene cluster including genes encoding homologs of cell-surface glycolipid-synthesis proteins and components of the type II protein secretion system (T2SS). To identify the genes involved in P49-selective protein transportation, we disrupted the genes in the cluster and analyzed the transportation of P49 to EMVs of the mutants. P49 of the mutants of the genes encoding components of the T2SS was localized mainly at the cellular fraction, not in the EMV fraction and the post-vesicle fraction removed EMVs from the culture supernatant. This result reveals that these homologs are components of a protein secretion machinery that plays an essential role in the transport of P49 to EMVs. Because P49 has an N-terminal signal sequence, the nascent protein synthesized in the cytoplasm is translocated across the inner membrane. Thus, it is assumed that the possible protein secretion machinery delivers P49 from the periplasm to the cell surface or extracellular space (Figure 1). Disruption of the genes encoding cell-surface polysaccharide-synthesis protein (Wzx2 and LptA), lipid-modification protein (GdpD), and nitroreductase (NfnB) changed the localization of P49. P49 of these mutants disappeared from EMVs and was found mainly from the PVF. On the other hand, it was also found that these genes are not essential for the EMV synthesis, suggesting that proteins encoded by these genes are required for the association of P49 with EMVs after its translocation to the cell surface or extracellular space. Wzx2 is a homolog of Wzx flippase family protein, which contributes to the biosynthesis of the O-antigen of lipopolysaccharides. Thus, it is hypothesized

that Wzx2 plays a role in the biosynthesis of a surface glycolipid of EMVs required for tethering of P49 to EMVs (Figure 1).

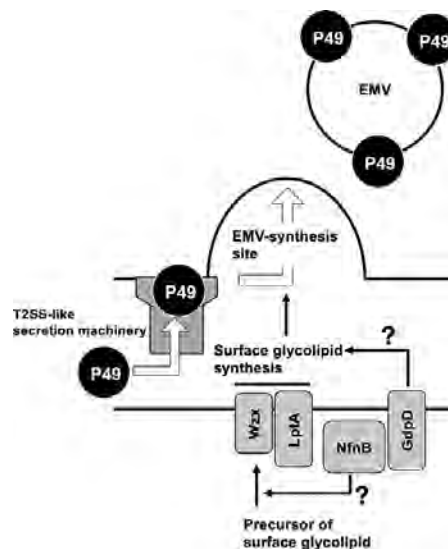


Figure 1. Possible model of P49-transportation pathway to EMVs of *Shewanella vesiculosa* HM13.

Detailed Analysis of Bacterial Bioconversion of DHA into EPA

Some marine microorganisms produce ω -3 polyunsaturated fatty acids such as eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA), which are beneficial to human health. To develop the microbial production system for EPA/DHA, their *de novo* biosynthesis has been intensively investigated. However, a comprehensive understanding of EPA/DHA metabolism including degradation and bioconversion is lacking. The EPA-producing bacterium *Shewanella livingstonensis* Ac10 is capable of not only biosynthesizing EPA-containing phospholipids but also converting exogenous DHA into EPA. We previously found that the unique conversion is mediated by an auxiliary β -oxidation enzyme, *i.e.* 2,4-dienoyl-CoA reductase. To further reveal the conversion mechanism, we examined the involvement of two homologs of acyl-CoA dehydrogenase (FadE1 and FadE2), which presumably catalyze the first step of β -oxidation reactions. Mutagenesis experiments demonstrated that the disruption of *fadE1*, but not of *fadE2*, led to the decreased DHA conversion. The expression of *fadE1* was enhanced when a cell was supplemented with DHA, while that of *fadE2* remained unchanged. Consistent with these *in vivo* results, we found that the recombinant FadE1 catalyzed the dehydrogenation of DHA-CoA *in vitro*. Altogether, these data suggest that FadE1 is a β -oxidation enzyme that contributes to the conversion from DHA to EPA.

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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 Polymer Properties
Self Assembly Softmatter
Hierarchical Structure



Selected Publications

Kishimoto, M.; Mita, K.; Ogawa, H.; Takenaka, M., Effect of Submicron Structures on the Mechanical Behavior of Polyethylene, *Macromolecules*, **53**, 9097-9107 (2020).
Ogawa, H.; Ono, S.; Nishikawa, Y.; Fujiwara, A.; Kabe, T.; Takenaka, M., Improving Grazing-incidence Small-angle X-ray Scattering-computed Tomography Images by Total Variation Minimization, *J. Appl. Cryst.*, **53**, 140-147 (2020).
Okamoto, M.; Mita, K.; Uekusa, T.; Takenaka, M.; Shibayama, M., Development of Elastic Recovering 4-methyl-1-pentene/propylene Copolymer, *Polymer*, **191**, [122269-1]-[122269-10] (2020).
Nishitsuji, S.; Watanabe, Y.; Takebe, T.; Fujii, N.; Okano, M.; Takenaka, M., X-ray Scattering Study on the Changes in the Morphology of Low-modulus Polypropylene Under Cyclic Uniaxial Elongation, *Polym. J.*, **5**, 279-287 (2020).

Effect of Submicron Structures on the Mechanical Behavior of Polyethylene

We investigated changes in the hierarchical structures of polyethylene (PE) during tensile testing by means of time-resolved ultra small-angle scattering (USAXS), small-angle, and wide-angle X-ray scattering. We discovered the enhancement of density fluctuation on the submicron scale by USAXS, which led to the generation of voids and necking. The spatial inhomogeneity of the stress fields associated with density or crystallinity fluctuation on the submicron scale induced the inhomogeneous flow during stretching. In other words, the change in the higher order structure than in the lamellar structure dominated the mechanical properties of PE. The enhancement of the fluctuation in linear low-density polyethylene (LLDPE) was smaller than that in high-density polyethylene (HDPE). Mechanical melting in the LLDPE suppressed the inhomogeneous flow and delayed the generation of voids and necking. As a result, the LLDPE exhibited two yield points on a S-S curve, while the HDPE exhibited one yield point. We believe that these results support the universality of the viscoelastic effect, which has been proposed to explain the fracture mechanisms of other systems such as semi-dilute polymer solutions and glassy materials.

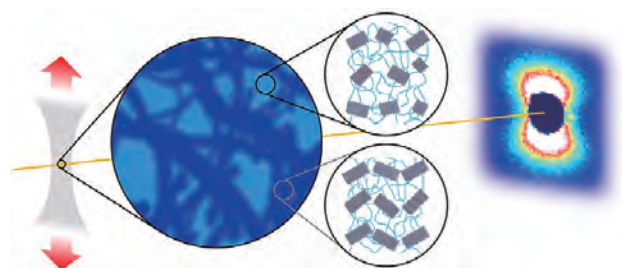


Figure 1. Schematic illustrations of the changes in the hierarchical structures in the PE during stretching.

Molecular Weight Effect on the Transition Process of Symmetric PS-*b*-P2VP during Spin-Coating

We studied the transition behavior in symmetric poly(styrene-*b*-2-vinyl pyridine) (PS-*b*-P2VP) with different molecular weights during spin-coating from a toluene solution by using grazing-incidence small-angle X-ray scattering (GISAXS). For the lowest molecular weight condition used here (the number-average molecular weight, M_n , was 16,500), the disordered micelles transitioned into disordered structures during evaporation. When $M_n = 50,000$, the micelles transitioned into hexagonally packed cylindrical structures parallel to the substrate and then into lamellar structures. The effect of selective solvent evaporation on the transition process became significant when M_n was larger than 84,000. For $M_n = 84,000$ and 199,000, the micelles first transitioned into spheres on the body-centered cubic lattice (BCC), where the BCC (110) plane was aligned perpendicular to the substrate. Then, the spheres coalesced into loosely packed cylindrical structures. The convection effect of the solvent caused this coalescence, and vitrification prohibited continued transitioning into the lamellar structures from the cylindrical structures. PS-*b*-P2VP with $M_n = 428,000$ self-assembled into loosely packed cylindrical structures perpendicular to the substrate; thin films were formed after the transition from micelles into BCC structures. However, the BCC (110) plane did become aligned perpendicular to the substrate because the high viscosity prevented alignment due to convection during the solvent evaporation.

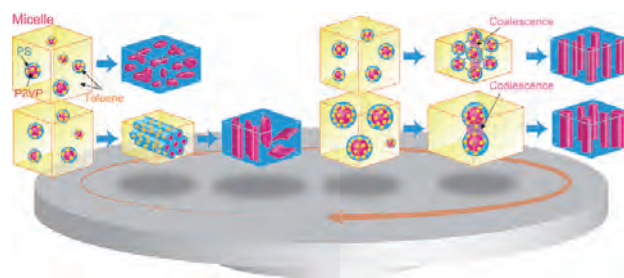


Figure 2. Schematic representation of the structural formation of PS-*b*-P2VP with molecular weights in the spin-coating process.

Division of Multidisciplinary Chemistry – Molecular Rheology –

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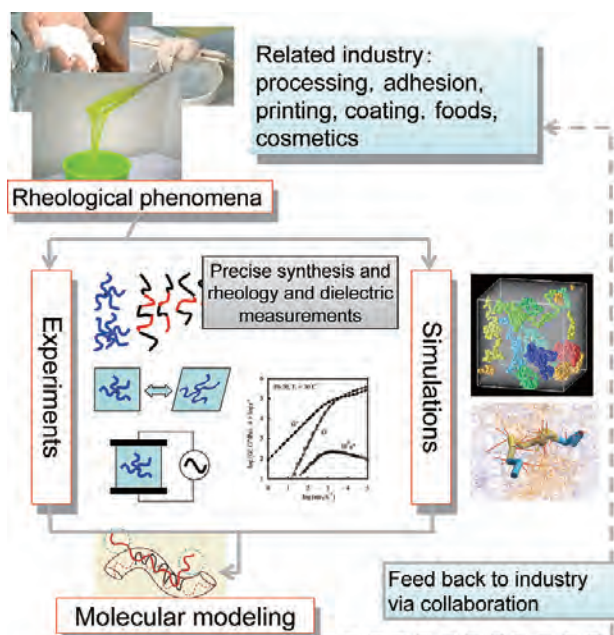
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Scope of Research

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.

KEYWORDS

Rheology Dielectric Spectroscopy Softmatter



Selected Publications

Iwakaki, H.; Urakawa, O.; Inoue, T.; Nakamura, Y.; Matsumiya, Y.; Watanabe, H., Rheo-Optical and Dielectric Study on Dynamics of Bottlebrush-like Polymacromonomer Consisting of a Polyisoprene Main Chain and Polystyrene Side Chains, *Macromolecules*, **53**, 7096-7106 (2020).

Matsumiya, Y.; Watanabe, H., Entanglement-Loosening Dynamics Resolved through Comparison of Dielectric and Viscoelastic Data of Type-A Polymers: A Review, *Rubber Chemistry and Technology*, **93**, 22-62 (2020).

Zhao, X.; Yu, W.; Matsumiya, Y.; Watanabe, H.; Kwon, Y., Dielectric Relaxation of Type-A Rouse Chains Undergoing Reversible End-Adsorption and Desorption, *J. Soc. Rheol. Jpn.*, **48**, 27-35 (2020).

Matsumiya, Y.; Watanabe, H.; Urakawa, O.; Inoue, T.; Kwon, Y., Effect of Head-to-Head Association/Dissociation on Viscoelastic and Dielectric Relaxation of Entangled Linear Polyisoprene: An Experimental Test, *Macromolecules*, **53**, 1070-1083 (2020).

Effect of Head-to-Head Association/Dissociation on Viscoelastic and Dielectric Relaxation of Entangled Linear Polyisoprene: An Experimental Test

For linear high-*cis* polyisoprene having a monofunctionally associative carboxyl group at the chain head (PI30-COOH; $M = 30.5 \times 10^3$), linear viscoelastic and dielectric behavior was examined in its entangled bulk system. The PI30-COOH unimer chain had type-A dipoles aligned from the tail to head so that its large-scale motion (over the tail-to-head distance) activated not only viscoelastic but also dielectric relaxation. Consequently, the head-associated dimer of PI30-COOH had symmetrically inverted type-A dipoles, and its large-scale motion also activated both viscoelastic and dielectric relaxation. These unimer and dimer were coexisting in the system at equilibrium because of the association/dissociation reaction at the carboxyl group, and this reaction strongly affected the viscoelastic and dielectric behavior. Experimentally, the reaction effect was examined by utilizing two reference polyisoprenes undergoing no reaction, PI30 and (PI30)₂: PI30 was a prepolymer of PI30-COOH before introducing the carboxyl group at the head, and (PI30)₂ was a head-to-head dimer of PI30 prepared by coupling of the PI30 anion. The viscoelastic and dielectric relaxation was found to be faster for the PI30-COOH system than for a reference PI30/(PI30)₂ blend having the unimer/dimer composition identical to that in the PI30-COOH system (determined from Fourier transform infrared measurement), and this difference between the PI30-COOH system and the blend was more significant for the viscoelastic relaxation than for the dielectric relaxation. This experimental fact unequivocally indicates that the reaction induces motional coupling between the unimer and dimer to significantly affect the relaxation behavior of these chains. This result lends support to a recent model analyzing this coupling for entangled (reptating) unimer and dimer. In fact, the model described low-frequency asymptotes of the viscoelastic and dielectric losses of PI30-COOH surprisingly well, given that the viscoelastic and dielectric asymptotes of the reference PI30 bulk system were separately fitted by the model to determine the terminal relaxation times in the model calculation in the absence of reaction. This success of the model strongly suggests that the difference of the reaction effects on the dielectric and viscoelastic relaxation reflects the vectorial and tensorial nature of the

respective relaxation processes. The dielectric relaxation reflects the (vectorial) first-moment average of bond vectors \mathbf{u} of the chain so that the dipole inversion of the dimer leads to pairwise coupling of the dielectric modes of the unimer and dimer under the reaction, thereby allowing the reaction to affect the dielectric relaxation just moderately. In contrast, the viscoelastic relaxation detects the (tensorial) second-moment average of \mathbf{u} so that the reaction results in multiple coupling of the viscoelastic modes of the unimer and dimer to strongly affect the viscoelastic relaxation.

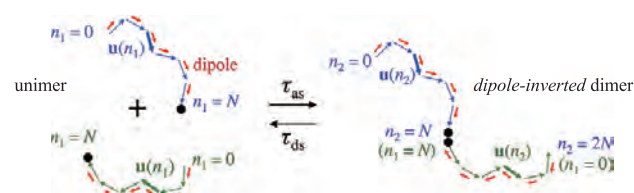


Figure 1. Illustration of head-to-head associating unimers and dissociating dimer at equilibrium. Purple circles at 0-th segments of the blue and green unimers (A and B) indicate the associative heads. The unimers and dimer have type-A dipoles aligned along the chain backbone without and with inversion, respectively.

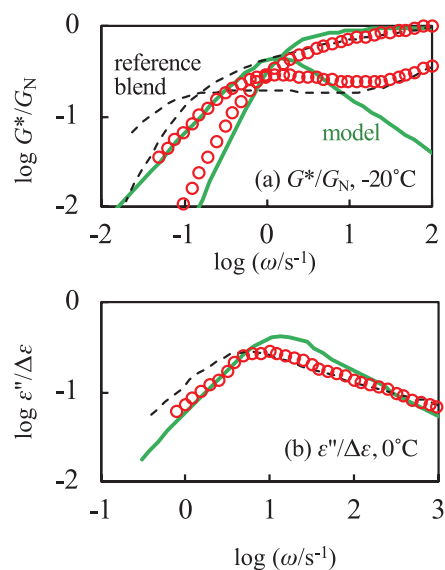


Figure 2. Comparison of (a) viscoelastic and (b) dielectric data (red circles) of PI30-COOH bulk system, model calculation (green solid curves), and data of the reference blend systems (thin dashed curves).

Division of Multidisciplinary Chemistry

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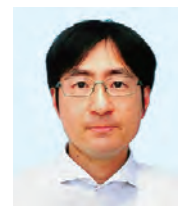
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Scope of Research

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



Selected Publications

Liu, J.; Ozaki, M.; Yakumar, S.; Handa, T.; Nishikubo, R.; Kanemitsu, Y.; Saeki, A.; Murata, Y.; Murdey, R.; Wakamiya, A., Lead-Free Solar Cells Based on Tin Halide Perovskite Films with High Coverage and Improved Aggregation, *Angew. Chem. Int. Ed.*, **57**, 13221-13225 (2018).
Truong, M. A.; Lee, J.; Nakamura, T.; Seo, J.-Y.; Jung, M.; Ozaki, M.; Shimazaki, A.; Shioya, N.; Hasegawa, T.; Murata, Y.; Zakeeruddin, S. M.; Gratzel, M.; Murdey, R.; Wakamiya, A., Influence of Alkoxy Chain Length on the Properties of Two-Dimensionally Expanded Azulene Core-Based Hole-Transporting Materials for Efficient Perovskite Solar Cells, *Chem. Eur. J.*, **25**, 6741-6752 (2019).
Ozaki, M.; Shimazaki, A.; Jung, M.; Nakaike, Y.; Maruyama, N.; Yakumar, S.; Rafieh, A. I.; Sasamori, T.; Tokitoh, N.; Ekanayake, P.; Murata, Y.; Murdey, R.; Wakamiya, A., A Purified, Solvent-Intercalated Precursor Complex for Wide Process Window Fabrication of Efficient Perovskite Solar Cells and Modules, *Angew. Chem. Int. Ed.*, **58**, 9389-9393 (2019).
Nakamura, T.; Yakumar, S.; Truong, M. A.; Kim, K.; Liu, J.; Hu, S.; Otsuka, K.; Hashimoto, R.; Murdey, R.; Sasamori, T.; Kim, H. D.; Ohkita, H.; Handa, T.; Kanemitsu, Y.; Wakamiya, A., Sn(IV)-free Tin Perovskite Films Realized by in situ Sn(0) Nanoparticle Treatment of the Precursor Solution, *Nat. Commun.*, **11**, 3008 (2020).
Nishimura, H.; Okada, I.; Tanabe, T.; Nakamura, T.; Murdey, R.; Wakamiya, A., Additive-free Cost-Effective Hole-Transporting Materials for Perovskite Solar Cells Based on Vinyl Triarylaminines, *ACS Appl. Mater. Interfaces*, **12**, 32994-33003 (2020).

Sn(IV)-Free Tin Perovskite Films Realized by in situ Sn(0) Nanoparticle Treatment of the Precursor Solution

The toxicity of lead perovskite hampers the commercialization of perovskite-based photovoltaics. While tin perovskite is a promising alternative, the facile oxidation of tin(II) to tin(IV) causes a high density of defects, resulting in lower solar cell efficiencies. Here, we show that tin(0) nanoparticles in the precursor solution can scavenge tin(IV) impurities, and demonstrate that this treatment leads to effectively tin(IV)-free perovskite films with strong photoluminescence and prolonged decay lifetimes. These nanoparticles are generated by the selective reaction of a dihydropyrazine derivative with the tin(II) fluoride additive already present in the precursor solution. Using this nanoparticle treatment, the power conversion efficiency of tin-based solar cells reaches 11.5%, with an open-circuit voltage of 0.76 V. Our nanoparticle treatment is a simple and broadly effective method that improves the purity and electrical performance of tin perovskite films.

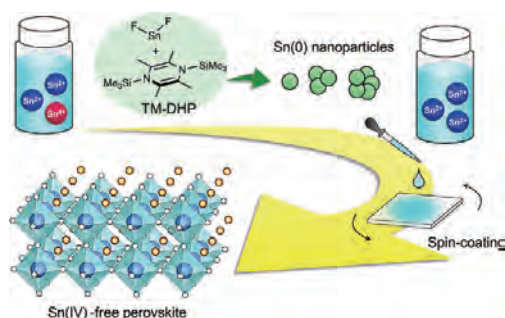


Figure 1. Schematic illustration of the Sn(IV) scavenging method to fabricate Sn(IV)-free perovskite films.

Hole-Transporting Polymers Containing Partially Oxygen-Bridged Triphenylamine Units and Their Application for Perovskite Solar Cells

A series of polymers composed of partially oxygen-bridged triphenylamine units was successfully synthesized by Suzuki-Miyaura or Migita-Kosugi-Stille cross coupling reactions. In addition to the polymer with directly connected triphenylamine units, **P1**, different π -spacers, were introduced into the polymer main chains including *m*-benzene, **P2**, *p*-benzene, **P3**, and bithiophene, **P4**. Photoelectron yield spectroscopy (PYS) results showed that the highest occupied molecular orbitals of these polymers lie above the valence bands of typical metal halide perovskites, suggesting efficient hole extraction from the perovskite. When used as hole-transporting materials in perovskite

solar cells, the maximum power conversion efficiency (PCE) of **P1–P4** reached 7.9% with LiTFSI additive, while the device of **P1** and **P4** without additive showed better PCE of 12.1% and 11.1%, respectively.

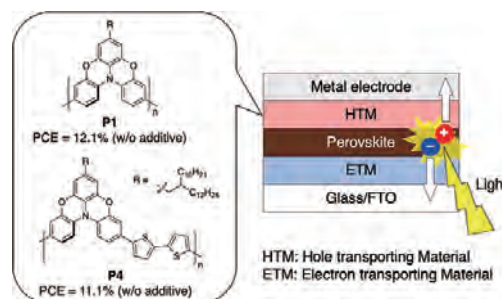


Figure 2. Development of hole-transporting polymers containing partially oxygen-bridged triphenylamine units.

Additive-Free, Cost-Effective Hole-Transporting Materials for Perovskite Solar Cells Based on Vinyl Triarylamines

A series of cost-effective hole-transporting materials (TOP-HTMs) for perovskite solar cells (PSCs) was designed and synthesized. The molecules, composed of multiple 4,4'-dimethoxytriphenylamines linked to a benzene core via *trans*-vinylene units, can be manufactured from inexpensive materials through a simple synthetic route. The photophysical, electrochemical, and thermal properties, as well as hole mobilities were strongly influenced by the position and number of vinyl triarylamine substituents on the core benzene ring. $\text{CH}_3\text{NH}_3\text{PbI}_3$ -based solar cells using the X-shaped TOP-HTM **3** with additives gave a high power conversion efficiency of 17.5% (forward scan) / 18.6% (reverse scan). Crucially, TOP-HTMs gave high working device efficiency without the need for conduction-enhancing additives. The power conversion efficiency for the device with additive-free TOP-HTM **3** was 16.0% (forward scan) / 16.6% (reverse scan). Device stability is also enhanced and is superior to the reference HTM, 2,2',7,7'-Tetrakis (*N,N*-di-*p*-methoxyphenylamine)-9,9'-spirobifluorene (Spiro-OMeTAD).

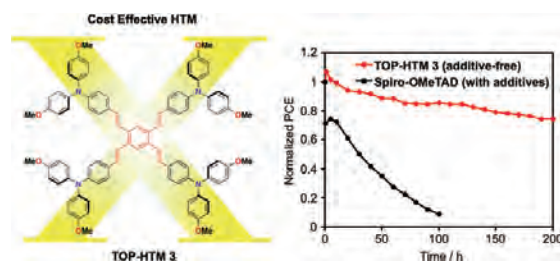


Figure 3. Chemical structure of X-shaped TOP-HTM **3** and the enhanced stability of perovskite solar cell device.

Advanced Research Center for Beam Science – Particle Beam Science –

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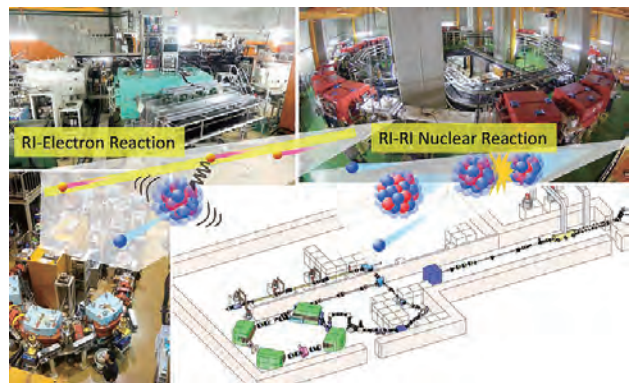
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Scope of Research

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 Accelerator Physics
Neutron Optics Storage Ring
Unstable Nuclear Physics



Selected Publications

Wakasugi, M.; Togasaki, M.; Ohnishi, T.; Kurita, K.; Toba, R.; Watanabe, M.; Yamada, K., FRAC: Fringing-RF-Field-Activated DC-to-Pulse Converter for Low-Energy Ion Beam, *Rev. Sci. Instrum.*, **89**, 095107 (2018).

Iwashita, Y.; Fuwa, Y.; Ishida, T.; Kino, K., Magnified Neutron Imaging with Modulating Permanent Magnet Sextupole Lens, *Proc. Int. Conf. Neutron Optics (NOP2017)*, **22**, [011008-1]-[011008-7] (2018).

Tsukada, K.; Enokizono, A.; Ohnishi, T.; Adachi, K.; Fujita, T.; Hara, M.; Hori, M.; Hori, T.; Ichikawa, S.; Kurita, K.; Matsuda, K.; Suda, T.; Tamae, T.; Togasaki, M.; Wakasugi, M.; Watanabe, M.; Yamada, K., First Elastic Electron Scattering from ^{132}Xe at the SCRIT Facility, *Phys. Rev. Lett.*, **118**, 262501 (2017).

Kitaguchi, M.; Iwashita, Y.; Shimizu, H. M., Concentration of the Velocity Distribution of Pulsed Neutron Beams, *Prog. Theor. Exp. Phys.*, **2017**, 043D01 (2017).

Kubo, T.; Iwashita, Y.; Saeki, T., Radio-frequency Electromagnetic Field and Vortex Penetration in Multilayered Superconductors, *Appl. Phys. Lett.*, **104**, 032603 (2014).

Developments of Charge Breeder for the Beam Recycling Technology

We promote the KAKEN-RNC collaboration to drive a new research field in unstable nuclear science. One of the attempts in the collaboration is a co-development of a beam recycling technique in a heavy-ion storage ring, which aims to a study of nuclear reaction especially for rarely-produced radio-active isotopes (RI) and RI-RI collision experiments. Unlike a conventional way using an extracted beam and a fixed target, the beam passing through the target without any reaction is recirculated in the ring and the accumulated beam hits the target turn by turn. We believe that the beam recycling technology will open up new research area such as an RI-RI collision experiment. Last year, the heavy-ion cooler storage ring (s-LSR) were moved from KAKEN to RIKEN RI Beam Factory (RIBF) for the R&D study. We will reconstruct s-LSR as a new storage ring named RUNBA (Recycled-Unstable Nuclear Beam Accumulator) which will be connected to the ISOL (Isotope Separator Online) system in RIBF as an RI beam injector.

One of the important techniques to be developed for the beam recycling is a charge breeder (CB) which is implemented between the ISOL and the RUNBA to convert the singly-charged ions to highly-charged ions. Due to a scarcity of RI, the conversion efficiency of the CB should be as high as possible. This year, a prototype of a resonant extraction CB (RECB) by which only desired charged state ions are selectively extracted was constructed as shown in Figure 1, and the performance study is ongoing.

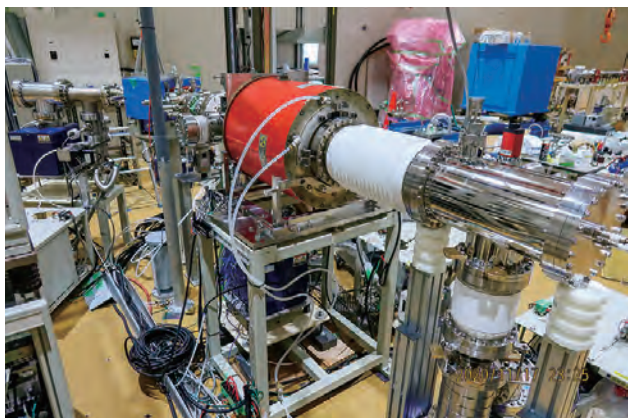


Figure 1. Prototype of Charge Breeder.

Renewal of KAKEN Accelerator Facility

We address some technical developments not only for the beam recycling but also for a nuclear physics measurement with KAKEN accelerators, namely an electron linac (KEL) and a storage ring (KSR). With a combination of KAKEN accelerators and a novel RI target forming technique developed at RIKEN ISOL facility, the photo-absorption cross sections of various nuclei including unstable ones will be measured by the virtual-photon tagging method. This is a unique and world's first way to access the giant resonance of unstable nuclei within a wide photon energy range.

This year, some maintenances and renewals of equipment of the KAKEN accelerator facility, such as an interlock system, an entrance and exit management system, a radiation safety system, and accelerator control systems have been done aiming to restart the facility from the next fiscal year because those systems were severely deteriorated by aging and some devices were broken. Figure 2 shows the renewed entrance and exit management system which controls the electronic lock and records when and who enters the controlled area by using a QR code. These works are supported by the International Joint Usage/Research Center and the Kyoto University President's Discretionary Fund.



Figure 2. Renewed Entrance and Exit Management System.

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

<http://laser.kuicr.kyoto-u.ac.jp/e-index.html>



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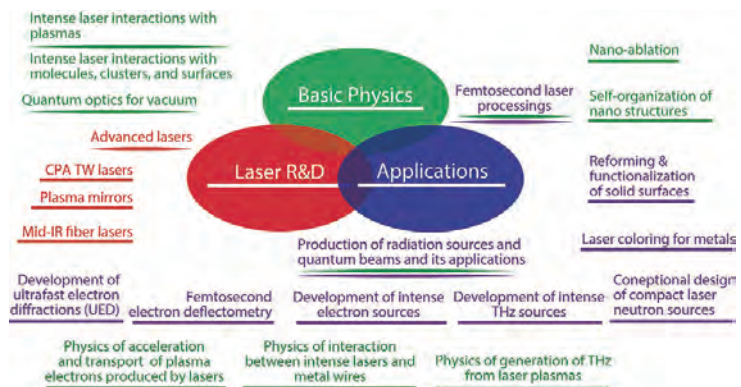
FURUKAWA, Yuki (D3) KONGO, Ryota (M2) TANAKA, Yohei (M2)

Scope of Research

The interaction of femtosecond laser pulses with matter involves interesting physics not seen with nanosecond laser pulses. Through investigations of the interaction physics, the potential of intense femtosecond lasers for new applications is being developed (e.g., laser-produced radiation and laser processing). Ultra-intense lasers can produce intense radiations (e.g., electrons, ions, and THz), which are promising as next-generation radiation sources. Ultra-short lasers can process any matter without thermal dissociation. Femtosecond laser processing is also the next-generation of laser processing. Our laboratory is equipped with an ultra-intense femtosecond laser named T6, to study the physics of intense laser–matter interactions and its applications.

KEYWORDS

Intense Laser Science
Laser Plasma Radiations (Electrons, Ions, and THz)
Ultrafast Electron Diffraction (UED)
Laser Nano-ablation Physics
Femtosecond Laser Processing



Selected Publications

- Inoue, S.; Sakabe, S.; Nakamiya, Y.; Hashida, M., Jitter-free 40-fs 375-keV Electron Pulses Directly Accelerated by an Intense Laser Beam and Their Application to Direct Observation of Laser Pulse Propagation in a Vacuum, *Sci. Rep.*, **10**, 20387 (2020).
- Hashida, M.; Furukawa, Y.; Inoue, S.; Sakabe, S.; Masuno, S.; Kusaba, M.; Sakagami, H.; Tsukamoto, M., Uniform LIPSS on Titanium Irradiated by Two-color Double-pulse Beam of Femtosecond Laser, *J. Laser Appl.*, **32**, 022054 (2020).
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Optical Properties of Titanium Induced by Below-ablation-threshold Irradiation

To understand the changes in the optical properties of a titanium surface induced by irradiation with low-intensity laser light that does not cause surface peeling, we have proposed a pump-and-probe method using femtosecond laser pulses with fluences below and above the ablation threshold (BAT and AAT, respectively). By analyzing the dependence of the ablation rate on the AAT probe-pulse fluence, the dynamical changes in the effective laser penetration depth and effective ablation threshold could be estimated. The dependences of the effective laser penetration depth and effective ablation threshold on the pump-pulse fluence F_{pump} below the ablation threshold F_{th} ($F_{\text{pump}} < F_{\text{th}}$) were measured with a delay of 100 ps. BAT irradiation with $F_{\text{pump}} > 0.18 F_{\text{th}}$ reduced both the effective laser penetration depth and effective ablation threshold compared with irradiation without the pump pulse. The obtained results also indicated a large reduction in the effective laser penetration depth (58% for $F_{\text{pump}} = 0.9 F_{\text{th}}$) and a small reduction in the effective ablation threshold (15% for $F_{\text{pump}} = 0.9 F_{\text{th}}$).

Uniform LIPSS on Titanium Irradiated by Two Color Double-pulse Beam of Femtosecond Laser

We have investigated the uniformity of laser-induced periodic surface structures (LIPSSs) generated on titanium surfaces irradiated with a two-color double-pulse cross-polarized beam with a time delay of $\Delta t = 0$ –200 ps. The double-pulse beam consisted of 800 nm pulses with a duration of 150 fs and 400 nm pulses with a duration of >150 fs. The fundamental-pulse fluence F_{800} and the second-harmonic pulse fluence F_{400} were set to be near the corresponding ablation thresholds of $F_{800\text{th}} = 0.108 \text{ J/cm}^2$ and $F_{400\text{th}} = 0.090 \text{ J/cm}^2$, respectively. We found that uniform LIPSSs could be produced on titanium surfaces using laser fluences of $1.5F_{400\text{th}} + 0.9F_{800\text{th}}$ and a delay of $\Delta t = 0$ –2 ps. The periodicity and direction of the LIPSSs were characterized by the wavelength and electric field of the fundamental (800 nm) pulse. The results suggest that the longer-wavelength pulse influences surface plasma wave generation and improves uniformity by the second harmonic pulse even though laser plasma is produced on the surface.

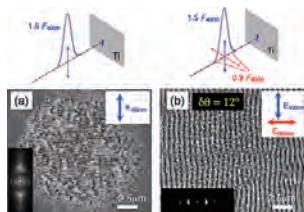


Figure 1. SEM images of titanium surfaces irradiated with (a) only the fundamental wavelength pulse with $N = 60$ pulses and (b) the two-color double-pulse beam with delay of $\Delta t = 0$ and $N = 60$ pairs of pulses. The LIPSS uniformity ($\delta\theta$) shows LIPSS characterized by the 800 nm pulse.

Generation of Jitter-free 40-fs 375 keV Electron Pulses Directly Accelerated by Intense Laser

In recent years, ultrafast science using ultrashort pulsed electrons with the high temporal and high spatial resolution has made rapid progress. Electrons with the energy of several hundred keV or less, short pulse width, and high brightness have succeeded in providing information that cannot be provided by other quantum probes in applications like ultrafast electron diffraction and electromagnetic field observation. For further development of these applications, namely for observation of more high-speed phenomena or irreversible phenomena with highly temporal-spatial resolutions, it is essential to shorten the pulses of electrons and further increase the amount of charge. In the development of ultra-short pulse electrons, which began with the generation of short-pulse electrons using a DC electron gun, it is a significant challenge to prevent the space charge effect which increasing the pulse width by self-generated electric fields. In order to overcome this problem essentially, the technique of electron pulse compression with RF cavity as a temporal-lens has been introduced, and this technology has been a great success, providing sub pC, several hundred fs electron pulses. When conducting pump-probe experiments with high time resolution using pulse compressed electrons, the critical parameter is not only the pulse width of the electron pulse. The timing jitter of the pump pulse and electron pulse as the probe pulse is also significant. No matter how short the probe pulse can be generated, if the time origin is not clear, high time resolution cannot be obtained when observing ultrafast phenomena. However, these methods use high-frequency electric fields in pulse compression, and jitter cannot be completely eliminated. This problem remains a very critical problem when using relatively slow electrons. In this work, we report the generation of ultrashort pulse electrons with extremely low timing jitter with a static field type compressor. By using electrons that are directly accelerated by shooting a solid thin film with an intense femtosecond laser, and using a pulse compression method with a phase rotator using permanent magnets, ultrashort electron pulses with extremely low timing jitter and short pulse width have been achieved. The number of electrons measured was 20 fC, the pulse width was 38 fs in RMS, and the long-term timing jitter was 14 fs in RMS. By adopting the electron pulse compression method using only the static field, the timing jitter is essentially zero. Therefore, we have succeeded in creating electron pulses that are extremely robust against external fluctuations. In addition, by generating electron pulses from the laser-plasma, there is no need to consider degradation and damage of photocathode limiting the amount of the number of electrons.

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Scope of Research

We study crystallographic and electronic structures of materials and their transformations through direct imaging of atoms or molecules by high-resolution electron spectromicroscopy, which realizes energy-filtered imaging and electron energy-loss spectroscopy as well as high-resolution imaging. By combining this with scanning probe microscopy, we cover the following subjects: 1) direct structure analysis, electron crystallographic analysis, 2) elemental analysis and electronic states analysis, 3) structure formation in solutions, and 4) epitaxial growth of molecules.



KEYWORDS

STEM-EELS ELNES Brownmillerite CTM4XAS Crystal Field Multiplet Calculation

Selected Publications

Saito, H.; Kurata, H., Formation of a Hybrid Plasmonic Waveguide Mode Probed by Dispersion Measurement, *J. Appl. Phys.*, **117**, [133107-1]-[133107-7] (2015).

Haruta, M.; Hosaka, Y.; Ichikawa, N.; Saito, T.; Shimakawa, Y.; Kurata, H., Determination of Elemental Ratio in an Atomic Column by Electron Energy-Loss Spectroscopy, *ACS Nano*, **10**, 6680-6684 (2016).

Haruta, M.; Fujiyoshi, Y.; Nemoto, T.; Ishizuka, A.; Ishizuka, K.; Kurata, H., Atomic-Resolution Two-Dimensional Mapping of Holes in the Cuprate Superconductor $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4+\delta}$, *Phys. Rev. B*, **97**, [205139-1]-[205139-5] (2018).

Yamaguchi, A.; Haruta, M.; Nemoto, T.; Kurata, H., Probing Directionality of Local Electronic Structure by Momentum-Selected STEM-EELS, *Appl. Phys. Lett.*, **113**, [053101-1]-[053101-4] (2018).

Haruta, M.; Fujiyoshi, Y.; Nemoto, T.; Ishizuka, A.; Ishizuka, K.; Kurata, H., Extremely Low Count Detection for EELS Spectrum Imaging by Reducing CCD Read-out Noise, *Ultramicroscopy*, **207**, [112827-1]-[112827-6] (2019).

Extraction of the Local Coordination and Electronic Structures of FeO₆ Octahedra Using Crystal Field Multiplet Calculations Combined with STEM-EELS

The material properties of metal oxides are sensitive to cation doping. The local atomic structure around such doped cations will be different from that in the bulk. The present work explores the extraction of the local structure of a minority component contained in an atomic column by analyzing the Fe $L_{2,3}$ energy-loss near-edge structure (ELNES) of atomic-resolution monochromated electron energy-loss spectra (EELS) using crystal field multiplet (CFM) calculations by CTM4XAS program. The present study focused on brownmillerite-type compounds, which have a structure $A_2BB'O_5$ comprising alternating layers of BO_4 tetrahedra and $B'O_6$ octahedra.

Figure 1 shows the experimental and simulated Fe $L_{2,3}$ -ELNES acquired from several iron oxide materials. These spectra show different features reflecting variations in local electronic structures. The energy levels of the $3d$ state for a transition metal having D_{4h} distorted octahedral symmetry in the mean field approximation is described by the crystal field parameters Dq , Dt , and Ds in CTM4XAS. In the present research, the energy width between two peaks in the experimental L_3 spectrum was employed as the crystal field splitting (CFS) $\Delta E = E_{d_{x^2-y^2}} - E_{d_{yzd_{zx}}} = 10Dq + 3Ds - 5Dt$. The optimal crystal field parameters were decided by fitting between simulated and experimental spectra. Figure 2 presents a calculated energy diagram of the Fe $3d$ state at an octahedral site. As for $Ca_2Fe_2O_5$ (CFO) and $Sr_2Fe_2O_5$ (SFO), the diagram roughly agrees with the one calculated by density functional theory (DFT). We can obtain reliable information concerning CFS with atomic-level resolution from experimental spectra in conjunction with CFM calculations without using DFT. In addition, the crystal field parameters are related to the $B'-O$ bond lengths: $Dq = Ze^2\langle r^4 \rangle / (6a^5)$, $Ds = (2/21)Ze^2\langle r^4 \rangle (1/a^5 - 1/b^5)$, where a and b are the equatorial and axial $B'-O$ bond lengths, r is the coordinate of the d electron. The bond lengths were estimated by using the $Ze^2\langle r^4 \rangle$ value derived from the Dq ($\Delta E = 10Dq = 1.4$ eV) and the bond length (2.02 Å) of α - Fe_2O_3 . The aspect ratios were estimated without using $Ze^2\langle r^4 \rangle$: $b/a = (4Dq / (4Dq - 7Dt))^{1/5}$. Table I compares the bond lengths and the aspect ratios determined by neutron diffraction and EELS. The aspect ratios obtained from the EELS data correspond reasonably well to the neutron data. The present method can reproduce not only CFS with atomic resolution but also local bond lengths of octahedra in real space.

We subsequently applied the same analysis to the Fe

$L_{2,3}$ ELNES acquired from the octahedral B' sites in $Ca_2Fe_{1.07}Mn_{0.93}O_5$ (CFMO), where the atomic concentration of Fe was $14.4 \pm 0.2\%$. In such cases, the local structure for the FeO_6 octahedra will be different from that for the more common MnO_6 . The aspect ratio is close to that for CFO although the bond lengths are different. The difference is significant because the neutron results primarily reflect the MnO_6 octahedra. In contrast, the EELS results show the unique local structure of the FeO_6 octahedra present as a minor component in B' site. Thus, it is demonstrated that the present method is effective for investigating local structures around impurities.

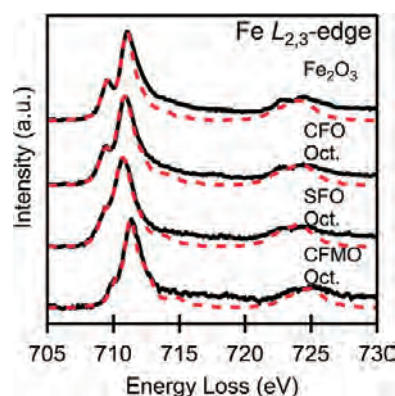


Figure 1. Fe $L_{2,3}$ -edge spectra acquired from α - Fe_2O_3 , $Ca_2Fe_2O_5$, $Sr_2Fe_2O_5$, and $Ca_2Fe_{1.07}Mn_{0.93}O_5$. Solid and dotted lines indicate experimental and simulated spectra, respectively. The energy range of fitting was 707–711.5 eV because the simulated spectra did not include the transitions to $4s$ and continuum states.

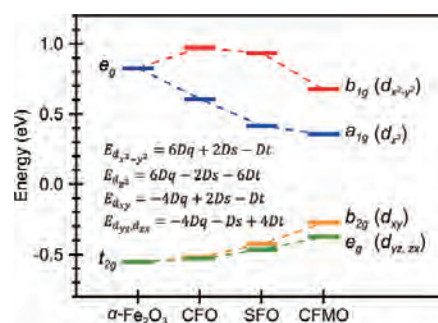


Figure 2. Energy diagram for the crystal field splitting of the Fe $3d$ state at an octahedral site.

Table I. The bond lengths obtained for various octahedra.

Sample	Bond	Neutron (Å)	EELS (Å)	Relative error (%)
$Ca_2Fe_2O_5$	a	1.97	2.00	1.4
	b	2.13	2.18	2.3
	b/a	1.08	1.09	1.0
$Sr_2Fe_2O_5$	a	1.98	2.04	2.8
	b	2.22	2.35	5.8
	b/a	1.12	1.16	3.6
$Ca_2Fe_{1.07}Mn_{0.93}O_5$	a	1.92	2.19	
	b	2.21	2.34	
	b/a	1.15	1.07	



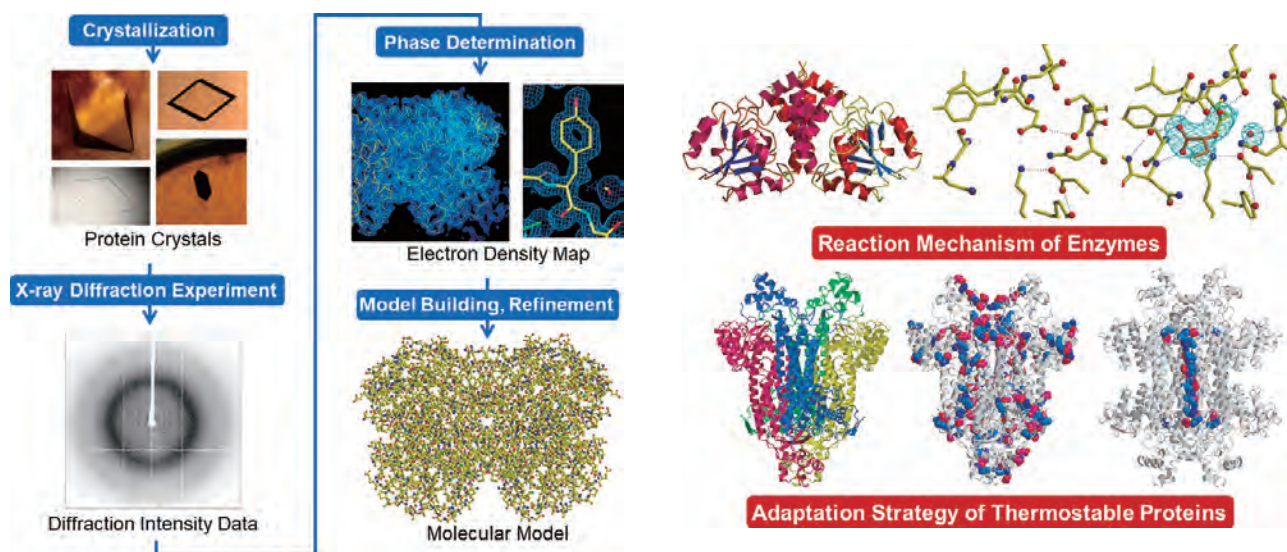
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Scope of Research

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 protein-protein 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



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).
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- 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).

Crystal Structure Analysis of the Oxygenase Component of Resorcinol Hydroxylase (GraA) in Complex with FAD and Nitrate Ions

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 small component, flavin reductase, generates reduced flavin for the oxygenase component to oxygenate the substrate. Thus, the enzymatic reaction is executed in two steps. However, hydroxylation activity is exhibited in the cooperative presence of both components. To understand the structural basis for the catalytic mechanism, we performed a crystal structure analysis of the oxygenase component (GraA) from *Rhizobium* sp. strain MTP-10005 in complex with FAD and nitrate ions. GraA is a tetramer, and its subunit consists of 409 amino acid residues.

The N-terminal His-tagged GraA was used for crystallization. The protein solution consisted of 12 mg/ml GraA, 1 mM FAD, 6 mM resorcinol, and 49 mM Tris-HCl pH 8.0. Crystals with suitable sizes for X-ray diffraction experiments were obtained in several days by a sitting drop vapor diffusion method with a reservoir solution consisting of 20% (w/v) PEG3350 and 0.2 M KNO₃. These crystals belonged to the monoclinic space group *C*2 with unit cell dimensions of $a = 155.4 \text{ \AA}$, $b = 102.8 \text{ \AA}$, $c = 128.2 \text{ \AA}$, $\beta = 104.6^\circ$. Diffraction data were collected up to 2.0 Å resolution under cryogenic conditions at beamline BL-1A, PF, Tsukuba, Japan. The structure was determined by molecular replacement and refined at 2.0 Å resolution.

In the crystal, a tetramer exists in the asymmetric unit and each subunit binds an FAD and a nitrate ion. GraA is a tetramer of four identical subunits related to one another by three molecular 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 FAD is located in the space encompassed by these three domains and binds to the polypeptide chains via hydrophobic and hydrophilic interactions. The loop region of 13 residues (residues Gly271–Asn283), which is

disordered in the apo-form structure, is ordered and covers the FAD of another subunit. The turn portion of the loop occludes the entrance of the active site. The nitrate ion and three water molecules bind to the active site via hydrogen bonds (Figure 3). Side chains of Tyr127, His364, Ser386, and Gln408 take part in the interactions. These residues might be involved in substrate binding or catalytic reactions.

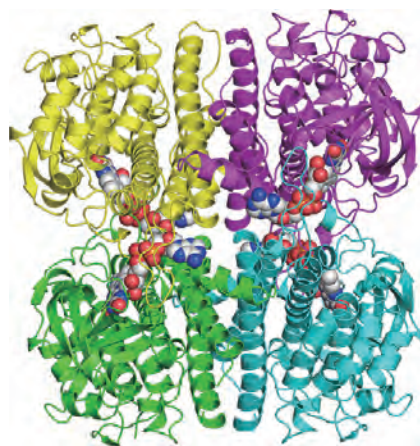


Figure 1. Tetrameric molecular structure of the oxygenase component of resorcinol hydroxylase (GraA) from *Rhizobium* sp. strain MTP-10005 in complex with FAD and nitrate ions.



Figure 2. Subunit structure of the oxygenase component of resorcinol hydroxylase (GraA) from *Rhizobium* sp. strain MTP-10005 in complex with FAD and nitrate ions.

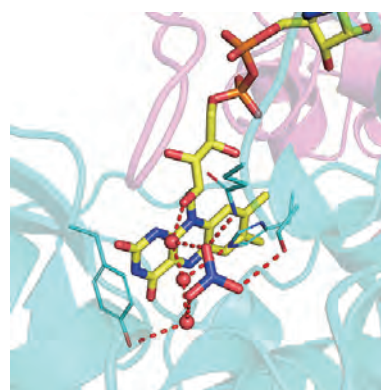


Figure 3. Structure of the active site of the oxygenase component of resorcinol hydroxylase (GraA) from *Rhizobium* sp. strain MTP-10005 in complex with FAD and nitrate ions.

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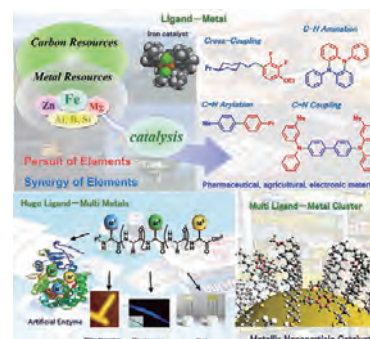
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Scope of Research

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 smart materials based on synergistic effect of various metals on artificial peptides (3) development of smart metallic nanoparticle catalysts based on supramolecular approaches (4) understanding of reaction mechanism of these catalytic reactions with the help of quantum chemical methods and synchrotron X-ray absorption spectroscopy.



KEYWORDS

Selective Organic Reaction Iron Catalyst Metalated Peptide Metallic Nanoparticle Catalyst Solution-Phase XAS Analysis

Selected Publications

Aoki, Y.; Toyoda, T.; Kawasaki, H.; Takaya, H.; Sharma, A. K.; Morokuma, K.; Nakamura, M., Iron-Catalyzed Chemoselective C-N Coupling Reaction: A Protecting-Group-Free Amination of Aryl Halides Bearing Amino or Hydroxy Groups, *Asian J. Org. Chem.*, **9**, 372-376 (2020).
Agata, R.; Lu, S.; Matsuda, H.; Isozaki, K.; Nakamura, M., Regio- and Stereoselective Synthesis of 1,4-enynes by Iron-catalyzed Suzuki-Miyaura Coupling of Propargyl Electrophiles under Ligand-free Condition, *Org. Biomol. Chem.*, **18**, 3022-3026 (2020).
Iwamoto, T.; Mizuhata, Y.; Tokitoh, N.; Nakamura, M., Development of P- and N-chirogenic Ligands Based on Chiral Induction from a Phosphorous Donor to a Nitrogen Donor in Palladium Complexes, *Organometallics*, **39**, 1672-1677 (2020).
Kanazawa, Y.; Mitsudome, T.; Takaya, H.; Hirano, M., Pd/Cu-Catalyzed Dehydrogenative Coupling of Dimethyl Phthalate: Synchrotron Radiation Sheds Light on the Cu Cycle Mechanism, *ACS Catal.*, **10**, 5909-5919 (2020).
Isozaki, K.; Taguchi, T.; Ishibashi, K.; Shimoaka, T.; Kurashige, W.; Negishi, Y.; Hasegawa, T.; Nakamura, M.; Miki, K., Mechanistic Study of Silane Alcoholysis Reactions with Self-Assembled Monolayer-Functionalized Gold Nanoparticle Catalysts, *Catalysts*, **10**, 908 (2020).

Iron-Catalyzed Cross-Coupling Reactions

Transition-metal-catalyzed carbon–carbon and carbon–heteroatom bond forming reactions are powerful tools for the synthesis of functional molecules. 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 recent representative examples, we developed the chemoselective iron-catalyzed C–N coupling reaction of diarylamines with protecting group-free haloanilines/halophenols (Figure 1a), which is of significant interest due to the applicability for the straightforward synthesis of protecting group-free intermediates for organic luminescent materials. By using DFT calculation, we proposed a catalytic cycle of dimeric-Fe-amide complex involving oxidative addition, 1,3-shift of halide anion, reductive elimination, and transmetalation steps (Figure 1b).

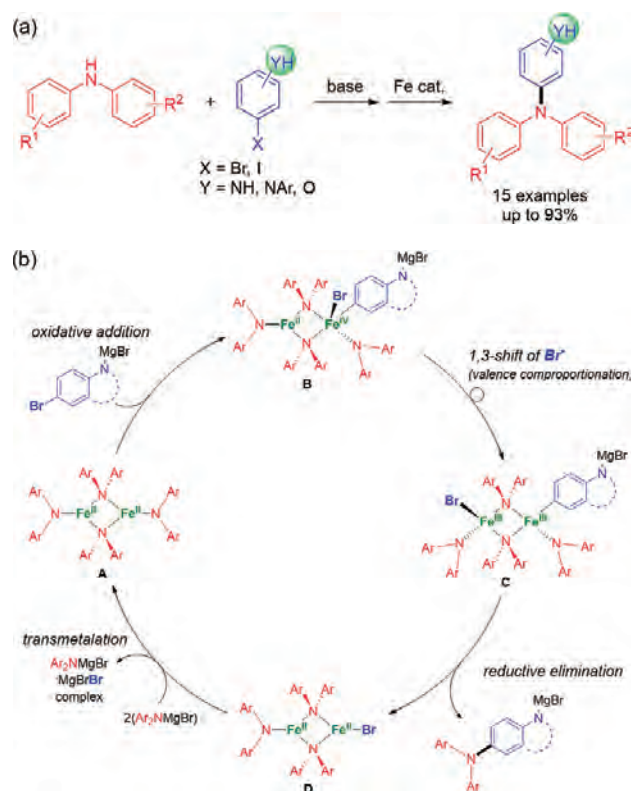


Figure 1. Iron-catalyzed chemoselective C–N coupling reaction with protecting group-free haloanilines and halophenols. (a) General reaction scheme and (b) a simplified plausible catalytic cycle.

Moreover, we developed ligand-free iron-catalyzed Suzuki–Miyaura coupling of lithium (*E*)- or (*Z*)-alkenylborates with propargyl electrophiles in stereospecific manner (Figure 2). The highly stereospecific nature of iron catalysis was demonstrated by the synthesis of tetrasubstituted 1,4-enyne, which has not been achieved by conventional catalytic methods.

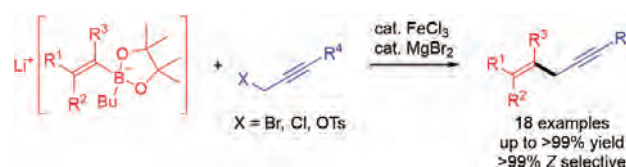


Figure 2. Iron-catalyzed Suzuki–Miyaura coupling of alkenylborates with propargyl electrophiles under ligand-free condition.

Novel Transition-Metal Catalyst Bound with Functional Amino Acid or Peptide

This project focuses on development of smart materials based on synergistic effect of various metals on artificial peptides. Based on this concept, we have developed novel ruthenium complex bound with norvaline, which catalyze efficient and selective oxidation of several methoxy-benzene analogues to quinones. Now we are trying further modification of the catalysts toward investigation of future chemical resources.

Supramolecular Approach for Creating Enhanced Catalysis of Metallic Nanoparticles

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.



International Research Center for Elements Science – Advanced Solid State Chemistry –

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School of Environmental and Chemical Engineering, Yanshan University, China, P.R., 12 December 2019–4 December 2020

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 Functional Transition Metal Oxides
Epitaxial Thin Film Growth High Pressure Synthesis



Selected Publications

Tan, Z.; Denis Romero, F.; Saito, T.; Goto, M.; Amano Patino, M. E.; Koedtruad, A.; Kosugi, Y.; Chen, W.-T.; Chuang, Y.-C.; Sheu, H.-S.; Attfield, J. P.; Shimakawa, Y., Charge Disproportionation and Interchange Transitions in Twelve-Layer BaFeO₃, *Phys. Rev. B*, **102**, 054404 (2020).

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Denis Romero, F.; Amano Patino, M. E.; Haruta, M.; Kurata, H.; Attfield, J. P.; Shimakawa, Y., Conversion of a Defect Pyrochlore into a Double Perovskite via High-Pressure, High-Temperature Reduction of Te⁶⁺, *Inorg. Chem.*, **59**, 343-349 (2020).

Charge Disproportionation and Interchange Transitions in Twelve-Layer BaFeO₃

Among compounds containing the high valent Fe ions, BaFeO₃ is of particular interest because several polymorphic phases with differently connected Fe⁴⁺O₆ octahedra are known (Figure 1). The simple cubic perovskite BaFeO₃, which is synthesized by low-temperature topochemical oxidation of BaFeO_{2.5}, consists of cubic close-packed layers (c) in a stacking sequence ...ccc...(3C), as shown in Figure 1a. When BaFeO₃ is synthesized at high temperature and ambient pressure, the six-layer hexagonal [6H, Figure 1b] polymorph is obtained. This consists of corner-sharing and face-sharing octahedra with the stacking sequence of ...cchcch... (*h* = hexagonal close-packed layer). A rhombohedral 12-layer compound (12R) with the stacking sequence ...cchhcchhcch... [Figure 1c] was also reported in oxygen-deficient BaFeO_{3.δ} (δ~0.1) obtained by high-pressure and high-temperature oxidation of brownmillerite BaFeO_{2.5}. The structure can also be considered as one where additional *h* layers are introduced into the 6H BaFeO₃ arrangement.

Here we investigated the structural and magnetic properties of fully oxygen stoichiometric BaFeO₃ containing unusually high valence Fe⁴⁺, leading to the discovery of a remarkable sequence of electronic and magnetic transitions on cooling; 2Fe⁴⁺ → Fe³⁺ + Fe⁵⁺ charge disproportionation and ordering over two sites accompanied by a structural distortion at 500 K; charge disproportionation of the remaining Fe⁴⁺ with magnetic order at 280 K; and an unprecedented charge interchange where Fe³⁺ and Fe⁵⁺ states are exchanged between two sites with spin orientation change at 50 K. Such successive charge disproportionation and interchange transitions with all charges fully ordered in each phase may result from the presence of both corner-sharing and face-sharing octahedra. The 12-layer BaFeO₃ demonstrates possibilities within the rich variety of transitions in charge-lattice-spin coupled systems.

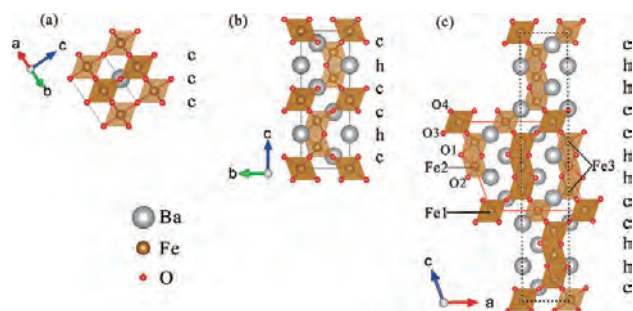


Figure 1. Crystal structures of (a) 3C, (b) 6H, and (c) 12-layer BaFeO₃.

Electric Field Induced Modulation of Transverse Resistivity Anomalies in SrRuO₃ Epitaxial Films

Perovskite strontium ruthenate SrRuO₃ (SRO) is an itinerant ferromagnet whose anomalous Hall effect (AHE) is dominantly contributed by the Berry curvature. Recently, ultrathin films of SRO were reported to exhibit anomalies in transverse (Hall) resistivity r_{xy} that were seen as hump structures (referred to as hump resistivity, ρ_{hump}) in the magnetic-field dependence of r_{xy} . The anomalies cannot be explained by the conventional framework of AHE and are often attributed to the emergence of the topological Hall effect (THE) due to formations of topologically nontrivial magnetic textures such as skyrmions. However, such topological magnetic textures have not been experimentally observed for SRO films and the origin of the anomalies (or ρ_{hump}) has been under debate. In fact, alternatives to the topological interpretation of the anomalies have been proposed. As shown in Figure 2, inhomogeneity in coercive field (H_c) and r_{AHE} (coexistence of positive and negative r_{AHE}) has been shown to explain the emergence of hump structures in the r_{xy} - H curves (or ρ_{hump}).

Here we show that the ρ_{hump} in the SRO channel layers in the field-effect transistor structures are modulated by applied gate voltages V_G . The applications of positive and negative V_G , respectively, increase and decrease ρ_{hump} . In addition, the V_G -induced changes in ρ_{hump} are essentially the same as those of the saturated ρ_{AHE} . These observations indicate that the transverse resistivity anomalies emerge because of the coexistence of the anomalous Hall resistivity with distinct mechanisms, *i.e.*, intrinsic and extrinsic ρ_{AHE} . Topological interpretation for ρ_{hump} such as formations of topologically nontrivial magnetic structures is not necessary. Furthermore, the V_G -induced changes in ρ_{hump} are dominated by the intrinsic ρ_{AHE} while the extrinsic ρ_{AHE} remains unchanged under the V_G applications. Our results reveal that electric field induced changes in the anomalous Hall effect depend on its mechanism.

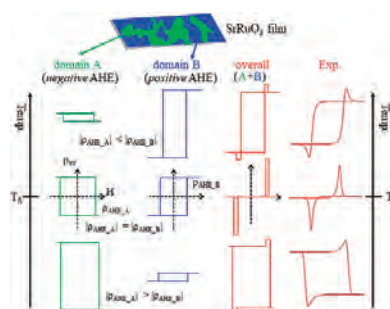


Figure 2. Schematics of the alternative model for transverse resistivity anomalies (hump resistivity, ρ_{hump}) in SrRuO₃.



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Scope of Research

This laboratory aims to establish new synthetic methodologies and new functional materials by designing well-defined catalysts based on transition metal chemistry. New concepts and ideas of molecular-based catalysts are accumulated by mechanistic investigations using experimental methods such as spectroscopy and kinetic techniques, as well as theoretical methods. The research subjects include: 1) development of novel organotransition metal systems for catalysis based on precise ligand design, and 2) preparation of π -conjugated polymers using direct arylation.

KEYWORDS

Transition Metal Complex
Homogeneous Catalyst
Reaction Mechanism
Low-coordinate Phosphorus Ligand
 π -Conjugated Polymer



Selected Publications

Wakioka, M.; Nakamura, Y.; Montgomery, M.; Ozawa, F., A Remarkable Ligand Effect of $P(2\text{-MeOC}_6\text{H}_4)_3$ on Palladium-Catalyzed Direct Arylation, *Organometallics*, **34**, 198-205 (2015).

Iizuka, E.; Wakioka, M.; Ozawa, F., Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization: Effective Prevention of Structural Defects Using Diamines, *Macromolecules*, **49**, 3310-3317 (2016).

Wakioka, M.; Takahashi, R.; Ichihara, N.; Ozawa, F., Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization: Highly Selective Synthesis of π -Conjugated Polymers with Diketopyrrolopyrrole Units, *Macromolecules*, **50**, 927-934 (2017).

Wakioka, M.; Ozawa, F., Highly Efficient Catalysts for Direct Arylation Polymerization (DArP), *Asian J. Org. Chem.*, **7**, 1206-1216 (2018).

Wakioka, M.; Morita, H.; Ichihara, N.; Saito, M.; Osaka, I.; Ozawa, F., Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization: Synthesis of Donor-Acceptor Polymers Containing Unsubstituted Bithiophene Units, *Macromolecules*, **53**, 158-164 (2020).

Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization: Synthesis of Donor–Acceptor Polymers Containing Unsubstituted Bithiophene Units

The combined use of P(2-MeOC₆H₄)₃ (**L1**) and TMEDA as ligands effectively prevents defect formation in palladium-catalyzed direct arylation polymerization (DARp) to give donor-acceptor type alternating copolymers (DA polymers) with unsubstituted 2,2'-bithiophene units (Figure 1). When only **L1** is used as the ligand, the reaction of **1a-Br** with 2,2'-bithiophene (**2-H**) in toluene at 100 °C forms a notable amount of insoluble materials via branching and cross-linking. In contrast, in the presence of **L1** and TMEDA, the formation of insoluble materials is completely suppressed, and poly(**1a-alt-2**) with well-controlled structure and high molecular weight is obtained ($M_n = 88,100$). Similarly, the reaction of **1b-Br** with **2-H** in toluene at 110 °C forms poly(**1b-alt-2**) with $M_n = 43,800$. The resulting polymers function as good components of bulk-heterojunction type organic solar cells (OSCs) using PC₇₁BM. In particular, poly(**1b-alt-2**) exhibits the best performance among DARp polymers reported so far (power conversion efficiency (PCE) = 9.0(1)%).

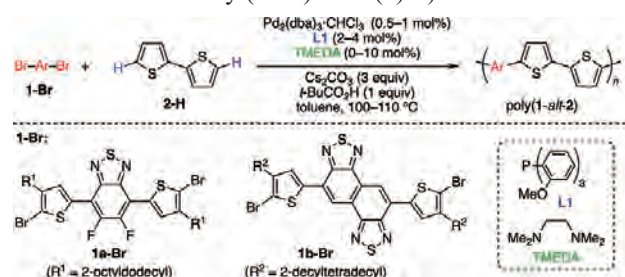


Figure 1. DARp synthesis of DA polymers containing bithiophene units.

Donor–Acceptor Polymers Containing 4,8-Dithienylbenzo[1,2-*b*:4,5-*b'*]dithiophene for Organic Solar Cells via Highly Selective Direct Arylation Polymerization

As shown above, recently, we have developed a highly selective catalyst that produces donor–acceptor-type alternating copolymers (DA polymers) with well-controlled structure via direct arylation polymerization (DARp). This method, however, often forms branching and cross-linking defects via undesirable C–H bond activation. These defects negatively impact device performance. In this new study, we the mixed-ligand catalyst shown above for the synthesis of DA polymers containing 4,8-dithienylbenzo[1,2-*b*:4,5-*b'*]dithiophene (DTBDT) units, which are known to function as excellent donors in DA polymers. The reaction of **3-Br** and **4-H** gives a DTBDT-containing

DA polymer (poly(**3-alt-4**)^{DARp}) having a well-controlled structure as it has homocoupling defects of 2.0%, which is much smaller than those of 14.8% for the Migita–Stille product (poly(**3-alt-4**)^{Stille}). poly(**3-alt-4**)^{DARp} functions as a good component of bulk-heterojunction type OSC using a non-fullerene acceptor (power conversion efficiency (PCE) up to 9.9%). The photovoltaic performance for poly(**3-alt-4**)^{DARp} is comparable to that for poly(**3-alt-4**)^{Stille} (PCE up to 9.8%).

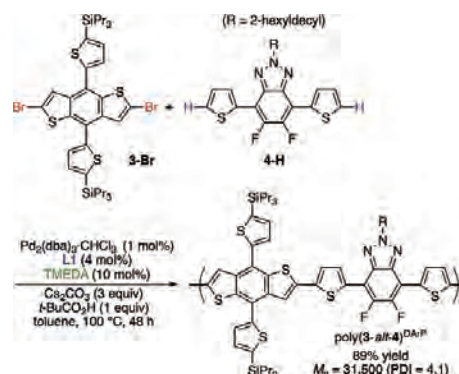


Figure 2. DARp synthesis of DA polymers containing 4,8-dithienylbenzo[1,2-*b*:4,5-*b'*]dithiophene units.

Synthesis and Properties of T-Shaped π -Conjugated Polymers

π -Conjugated polymers including poly(3-hexylthiophene) (P3HT) have attracted much attention due to their solution processability and good mechanical properties, which allow easy access to the next generation of large-area devices such as organic solar cells (OSCs) and perovskite solar cells (PSCs). To improve the performance of these devices, the π -conjugated polymers should adopt face-on orientation to the substrate, since the charges are generally transported through the intermolecular overlap of π -orbitals. Although a variety of polymers that exhibit face-on orientation have been found, the guiding principles for controlling the orientation of polymers have not yet been established. In this study, we examined T-shaped π -conjugated polymers composed of a thiazole-fused benzothiadiazole (TBT) core and three P3HT side-chains (**T-10** and **T-20**). We found that this molecular geometry could prevent the edge-on orientation and cause face-on orientation, as confirmed by 2D-GIXD.

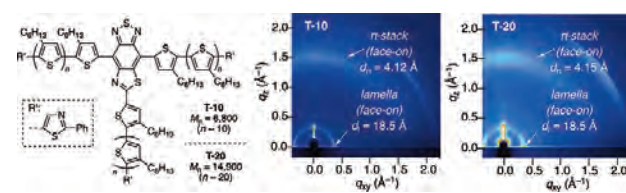


Figure 3. 2D-GIXD patterns of T-shaped π -conjugated polymers (**T-10** and **T-20**) in thin film.

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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 low-dimensional 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, and 3) photophysics of solar cell materials.



KEYWORDS

Femtosecond Laser Spectroscopy Single Photon Spectroscopy
Semiconductor Nanoparticles Perovskites
High Harmonic Generation

Selected Publications

Sanari, Y.; Otobe, T.; Kanemitsu, Y.; Hirori, H., Modifying Angular and Polarization Selection Rules of High-order Harmonics by Controlling Electron Trajectories in k-Space, *Nature Commun.*, **11**, [3069-1]-[3069-7] (2020).
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Sanari, Y.; Tachizaki, T.; Saito, Y.; Makino, K.; Fons, P.; Kolobov, A. V.; Tominaga, J.; Tanaka, K.; Kanemitsu, Y.; Hase, M.; Hirori, H., Zener Tunneling Breakdown in Phase-Change Materials Revealed by Intense Terahertz Pulses, *Phys. Rev. Lett.*, **121**, [165702-1]-[165702-6] (2018).
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Yamada, T.; Aharen, T.; Kanemitsu, Y., Near-Band-Edge Optical Responses of CH₃NH₃PbCl₃ Single Crystals: Photon Recycling of Excitonic Luminescence, *Phys. Rev. Lett.*, **120**, [057404-1]-[057404-6] (2018).

Origin of Negative Thermo-optic Coefficients of Lead Halide Perovskites

Lead halide perovskites are promising materials for flexible and efficient optoelectronic device applications. Recent studies have shown that the temperature dependence of their optical properties is quite different from that of conventional semiconductors. Understanding the origin of the unique temperature dependence is required from both fundamental physics and device application viewpoints. In this project, we clarified the temperature dependence of the refractive indices in lead halide perovskite $\text{CH}_3\text{NH}_3\text{PbCl}_3$. We found that $\text{CH}_3\text{NH}_3\text{PbCl}_3$ possesses negative thermo-optic coefficients for the entire visible wavelength region and its magnitude increases near the absorption edge. Analysis based on the Lorentz oscillator model revealed that the large thermal expansion coefficient leads to the large decrease in the valence electron density upon temperature rise, which consequently results in the unique negative thermo-optic coefficients.

Polarization Control of High-order Harmonics Induced by Two-color Orthogonally Polarized Laser Fields

Irradiation with a high-intensity laser pulse to a material causes light emission with a broad spectrum consisting of many harmonics of the excitation laser frequency. This phenomenon is called high-order harmonic generation (HHG). HHG has been actively studied toward new optical technologies, but the mechanisms of HHG are still under debate. In our experiments, in order to understand HHG mechanisms, a GaSe crystal was simultaneously excited by two orthogonally polarized optical pulses with wavelengths of $\lambda_1 = 2400$ nm and $\lambda_2 = 1300$ nm (Figure 1). We observed a broadband emission and multiple peaks originating from higher-order harmonic generation. Furthermore, it was clarified that the polarization of higher-order harmonics is determined by the motion of electrons that are strongly driven two-dimensionally by the electric field of orthogonal laser light. These results will lead not only to the technology for controlling the properties of high-order harmonics, but also to the ultrafast optoelectronics controlled by the electric field of laser light.

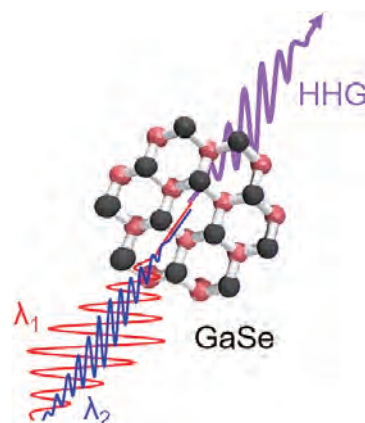


Figure 1. Experimental setup. Two orthogonally polarized pulses are focused on the sample.

Improvement of Optical Gain in Halide Perovskite Nanocrystals by Double Pump Method

Lead halide perovskite nanocrystals are expected for light-emitting device materials because they have superior optical properties. They exhibit high photoluminescence quantum yields and emission wavelength tunability by controlling the particle size and halide composition. However, a reabsorption process caused by exciton-exciton interactions suppresses the optical gain in photoexcited nanocrystal ensembles. This is one of the serious problems for realizing nanocrystal-based lasers. We evaluated the reabsorption process and the optical gain threshold of CsPbI_3 nanocrystals by double-pump transient absorption spectroscopy. Our study revealed that the efficient generation of asymmetric-hot biexciton states by the double-pump method is beneficial to suppress the reabsorption process and reduce the optical gain threshold (Figure 2).

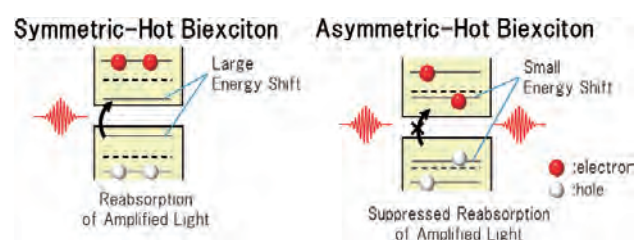


Figure 2. Schematics of the reabsorption processes in a symmetric-hot biexciton and an asymmetric-hot biexciton.

Bioinformatics Center – Chemical Life Science –

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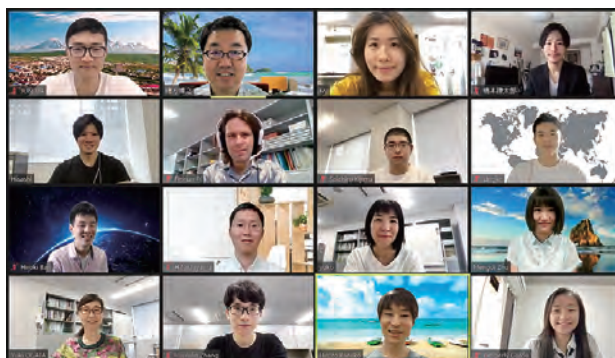
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Scope of Research

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

Selected Publications

Endo, H.; Blanc-Mathieu, R.; Li, Y.; Salazar, G.; Henry, N.; Labadie, K.; de Vargas, C.; Sullivan, M. B.; Bowler, C.; Wincker, P.; Karp-Boss, L.; Sunagawa, S.; Ogata, H., Biogeography of Marine Giant Viruses Reveals Their Interplay with Eukaryotes and Ecological Functions, *Nat. Ecol. Evol.*, doi: 10.1038/s41559-020-01288-w (2020).

Prodinger, F.; Endo, H.; Gotoh, Y.; Li, Y.; Morimoto, D.; Omae, K.; Tominaga, K.; Blanc-Mathieu, R.; Takano, Y.; Hayashi, T.; Nagasaki, K.; Yoshida, T.; Ogata, H., An Optimized Metabarcoding Method for Mimiviridae, *Microorganisms*, **8**, E506 (2020).

Sakurai, T.; Nishiyama, H.; Nagai, T.; Goto, S.; Ogata, H.; Kudo, M., Deficiency of Gankyrin in the Small Intestine is Associated with Augmented Colitis Accompanied by Altered Bacterial Composition of Intestinal Microbiota, *BMC Gastroenterol.*, **20**, 12 (2020).

Nishiyama, H.; Endo, H.; Blanc-Mathieu, R.; Ogata, H., Ecological Structuring of Temperate Bacteriophages in the Inflammatory Bowel Disease-affected Gut, *Microorganisms*, **8**, E1663 (2020).

Sunagawa, S.; Acinas, S. G.; Bork, P.; Bowler, C.; Tara Oceans Coordinators; Eveillard, D.; Gorsky, G.; Guidi, L.; Iudicone, D.; Karsenti, E.; Lombard, F.; Ogata, H.; Pesant, S.; Sullivan, M. B.; Wincker, P.; de Vargas, C., Tara Oceans: Towards Global Ocean Ecosystems Biology, *Nat. Rev. Microbiol.*, **18**, 428-445 (2020).

Improving a Metabarcoding Method for *Mimiviridae* Ecological Analysis

Mimiviridae is a group of mostly eukaryotic phytoplankton infecting viruses with big virions and long genomes. The relevance of *Mimiviridae* in the ecology of marine environments has been increasingly recognized by metagenomics based studies. We previously proposed a meta-barcoding approach based on 82 degenerate primer pairs (MEGAPRIMER) targeting the DNA polymerase gene of *Mimiviridae* to enable ecological profiling of *Mimiviridae*. Even though this method detected many operational taxonomic units (OTUs), it required large quantities of DNA and was laborious. Recently, we examined coastal seawater samples using varying PCR conditions and purification protocols to streamline the MEGAPRIMER method. The biggest advantage of our newly conceptualized methods are “primer cocktails”. We mixed several different primer pairs before PCR amplification and thereby reduced the required amount of environmental DNA by up to 90%, while reproducing the results of the original protocol. We compared and critically assessed the outcome of the different meta-barcoding approaches with quantifications using qPCR for selected OTUs. The quality control of MEGAPRIMER amplicon sequencing performed in this study solidified the MEGAPRIMER method as a new tool for ecological analysis of giant marine viruses. These newly developed MEGAPRIMER protocols will be especially useful for ecological analysis of a larger set of environmental samples.

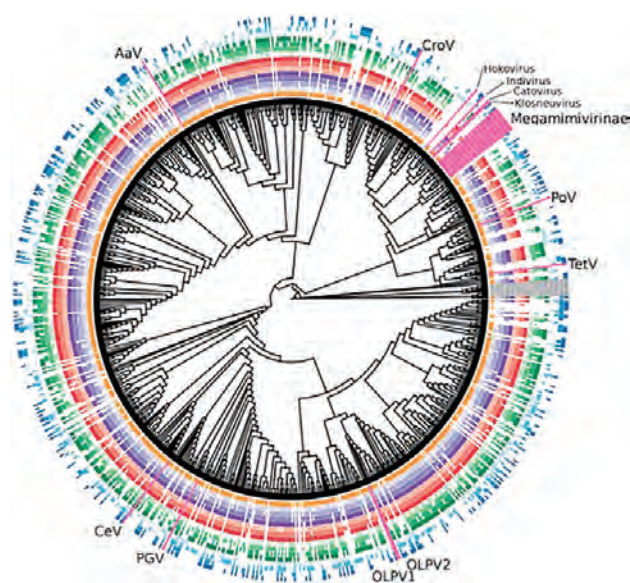


Figure 1. Phylogenetic tree of *Mimiviridae* OTUs found in different samples. Several OTUs that were closely related to isolated *Mimiviridae* were found.

Biogeography of Giant Viruses in the Global Ocean

Nucleocytoplasmic large DNA viruses (NCLDV, so called “giant viruses”) are thought to be ubiquitous in marine environments and infect diverse eukaryotes. However, their biogeography and ecology have yet to be explored at a global scale. By leveraging the *Tara* Oceans pole-to-pole metagenomic data, we investigated the distribution of NCLDV across size fractions, depths and biomes, as well as their associations with eukaryotic communities. Our analyses revealed a heterogeneous distribution of NCLDV across oceans, with an elevated uniqueness in polar biomes. Community structures of individual NCLDV families were found to be correlated with those of specific eukaryotic lineages such as chlorophytes, haptophytes, and choanoflagellates, suggesting clade specific geographical associations between NCLDV and host lineages (Figure 2). NCLDV communities were generally distinct between surface and mesopelagic zones, but exhibited a high similarity between the two depths at some locations. This vertical connectivity was correlated to surface phytoplankton biomass but not to physical mixing processes, suggesting the potential role of vertical export in structuring mesopelagic NCLDV communities. These results underscore the importance of the coupling between NCLDV and eukaryotes in biogeochemical processes in the ocean.

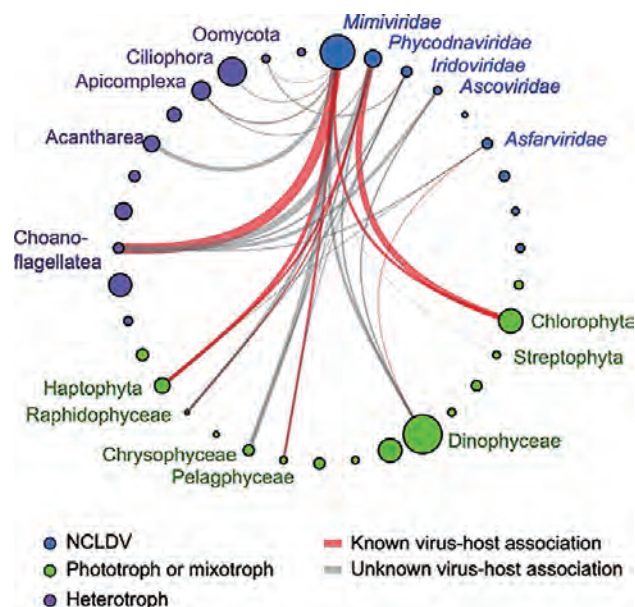


Figure 2. Associations between NCLDV and eukaryotic lineages as estimated by their distributions.

Bioinformatics Center

– Mathematical Bioinformatics –

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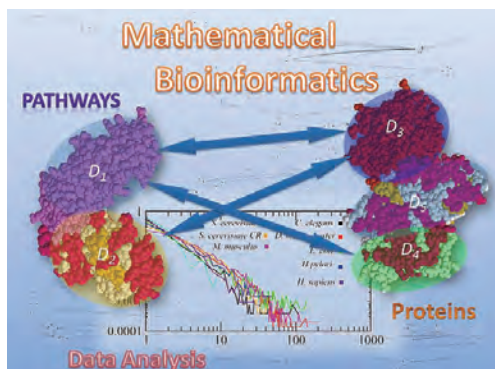
YANG, Ziwei (RS)

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



Selected Publications

Liu, P.; Melkman, A. A.; Akutsu, T., Extracting Boolean and Probabilistic Rules from Trained Neural Networks, *Neural Netw.*, **126**, 300-311 (2020).

Akutsu, T.; Melkman, A. A.; Tamura, T., Improved Hardness of Maximum Common Subgraph Problems on Labeled Graphs of Bounded Treewidth and Bounded Degree, *International Journal of Foundations of Computer Science*, **31**, 253-273 (2020).

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Zhu, J.; Wang, C.; Shurbevski, A.; Nagamochi, H.; Akutsu, T., A Novel Method for Inference of Chemical Compounds of Cycle Index Two with Desired Properties Based on Artificial Neural Networks and Integer Programming, *Algorithms*, **13**, [124-1]-[124-30] (2020).

Li, F.; Leier, A.; Liu, Q.; Wang, Y.; Xiang, D.; Akutsu, T.; Webb, G. I.; Smith, A. I.; Marquez-Lago, T.; Li, J.; Song, J., Procleave: Predicting Protease-Specific Substrate Cleavage Sites by Combining Sequence and Structural Information, *Genomics, Proteomics & Bioinformatics*, **18**, 52-64 (2020).

Algorithms for Extracting Boolean and Probabilistic Rules from Trained Neural Networks

Recent progress of deep learning technologies has demonstrated the power of artificial neural networks in making predictions in various areas. Therefore, it is important to develop a methodology for interpreting how a trained neural network arrives at its predictions.

We develop two algorithms to extracting rules from a trained neural network consisting of linear threshold functions. The first one extracts rules in the form of Boolean functions, and outputs much more concise rules, compared with an existing one, if the threshold functions correspond to 1-decision lists, majority functions, or certain combinations of these. The second one is based on dynamic programming and extracts probabilistic relations between the input values and the output value in the form of conditional probabilities. Although this problem is NP-hard (theoretically difficult) in general, the proposed algorithm works in pseudo-polynomial time if each hidden layer consists of a constant number of neurons. The potential usefulness of these two algorithms is demonstrated by conducting several computational experiments.

We have also been applying deep learning technologies to various problems in bioinformatics, which include cancer subtype classification, protein cleavage site prediction, RNA post-transcriptional modification site prediction, and lysine post-translational modification site prediction.

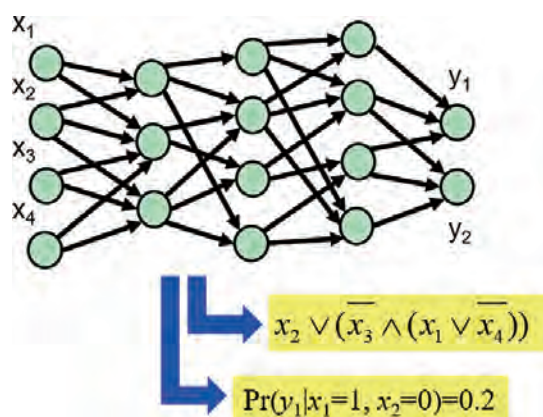


Figure 1. Our developed algorithms extract rules from trained neural networks in the forms of Boolean functions and conditional probabilities.

Grid-based Computational Methods for the Design of Constraint-based Parsimonious Chemical Reaction Networks to Simulate Metabolite Production: GridProd

Constraint-based metabolic flux analysis of knockout strategies is an efficient method to simulate the production of useful metabolites in microbes. Owing to the recent development of technologies for artificial DNA synthesis, it may become important in the near future to mathematically design minimum metabolic networks to simulate metabolite production.

We developed an efficient method for computing the design of minimum metabolic networks by using constraint-based flux balance analysis to simulate the production of useful metabolites. When the growth rate of this obtained parsimonious metabolic network is maximized, higher production rates are observed for many target metabolites when compared to existing methods. The set of reactions used in this parsimonious flux distribution consists of reactions included in the original genome scale model iAF1260. Under the conditions that the growth rate is maximized and the minimum cases of flux variability analysis are considered, the developed method produced more than 90% of metabolites, while the existing methods produced less than 50%.

The source code is freely available and is implemented in MATLAB and COBRA toolbox.

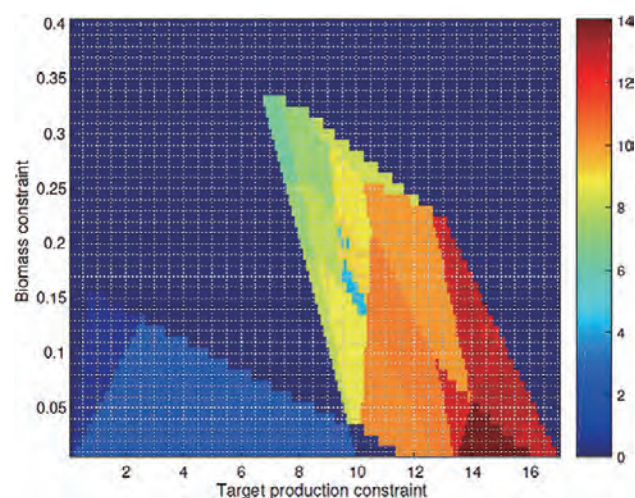


Figure 2. An example of the production rate heatmap for a target metabolite where each grid represents constraints for the ranges by the production rate and the growth rate.

Bioinformatics Center – Bio-knowledge Engineering –

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



Prof

MAMITSUKA, Hiroshi
(D Sc)



Senior Lect

NGUYEN, Hao Canh
(D Knowledge Science)

Student

NGUYEN, Duc Anh (D3)

Guest Res Assoc

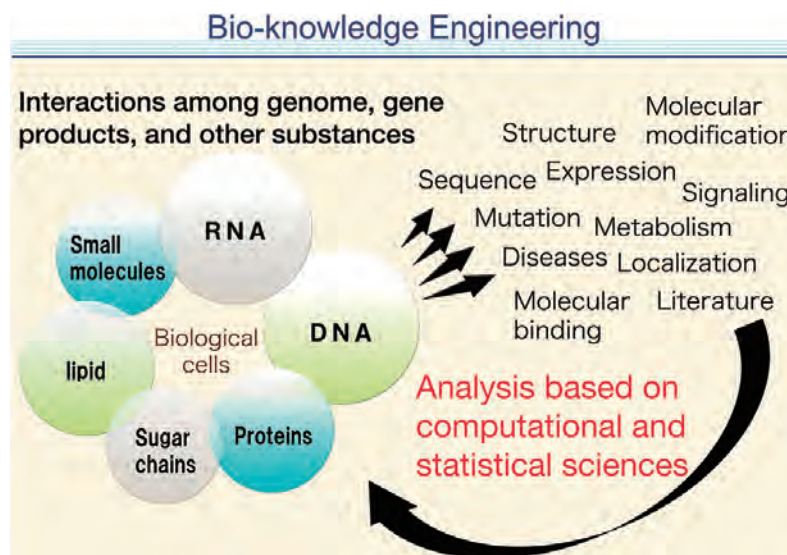
PETSCHNER, Peter (Ph D) Semmelweis University, Hungary, 28 November 2020– 27 November 2022

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
Computational Genomics
Data Mining
Machine Learning
Systems Biology



Selected Publications

Wimalawarne, K.; Yamada, M.; Mamitsuka, H., Scaled Coupled Norms and Coupled Higher-Order Tensor Completion, *Neural Computation*, **32**, 447-484 (2020).

Nguyen, C. H., Structured Learning in Biological Domain, *Journal of Systems Science and Systems Engineering*, **29**, 440-453 (2020).

Nakamura, A.; Takigawa, I.; Mamitsuka, H., Efficiently Enumerating Substrings with Statistically Significant Frequencies of Locally Optimal Occurrences in Gigantic String, *Proceedings of the AAAI Conference on Artificial Intelligence (AAAI 2020)*, **34(4)**, 5240-5247 (2020).

Nguyen, C. H.; Mamitsuka, H., Learning on Hypergraphs with Sparsity, *IEEE Transactions on Pattern Analysis and Machine Intelligence* (in press).

Wimalawarne, K.; Mamitsuka, H., Reshaped Tensor Nuclear Norms for Higher Order Tensor Completion, *Machine Learning* (in press).

Learning on Hypergraphs

Relational data has been of much interest in statistics and machine learning. It is the data with relationships among objects. To study this relational data, graph and hypergraph have been the main tools. Graph encodes relationships of pairs of objects. Hypergraph is a more general way of encoding high-order relationships, that is the relationship of variable numbers (two or more) of objects. It is a generalization of graph, in which only pairwise relationships can be represented. It finds applications in various domains where relationships of more than two objects are observed. In social networks, it can represent many groups of individuals that have common interests. In computer vision, it can represent patches of neighbor pixels that have similar colors. In bioinformatics, hypergraphs can be used to represent relationships among proteins in protein complexes, among sets of drugs and their side effects. In the example in Figure 1, we show a hypergraph that houses in the same street belongs to a set call a hyperedge. This is useful to study problem such as predicting house prices given various information including streets that the houses are located in.

On a hypergraph, as a generalization of graph, one wishes to learn a smooth function with respect to its topology. This is the semantics of graphs and hypergraphs in many domains. In social networks, individuals in the same academic groups might have interest in the same books. Patches of pixels with the same color in an image tends to belong to the same object in the image. Proteins in the same complex are likely to participate in the same cellular functionality. These observations have been formulated in statistics and machine learning, that labels of objects in the same given set (hyperedge) tend to be similar. Such a function is called *smooth on the graph/hypergraph*. It is a fundamental issue is to find suitable smoothness measures of functions on the nodes of a graph/hypergraph to make the function smooth.

There are various methods proposed to model hypergraphs. However, it is not clear why a method works for one problem, not for another problem. Strengths and weaknesses of the methods are hardly studied and poorly understood. In order to clarify all these methods, we show a

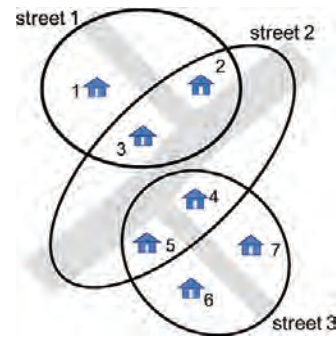


Figure 1. Houses on streets as nodes on hyperedges of a hypergraph.

general framework that generalizes all previously proposed smoothness measures on hypergraphs. Our framework not only allows for analyzing previous smoothness measures, but also gives rise to many new measures with useful properties. For example, we found that the commonly used total variation method to be too sensitive noises in data, which is very common in practice.

To address the problem of irrelevant or noisy data, we wish to incorporate sparse learning framework into learning on hypergraphs. From our proposed framework, we propose sparsely smooth formulations that learn smooth functions and induce sparsity on hypergraphs at both hyperedge and node levels. We show their properties and sparse support recovery results. This is one of the benefit of our framework to design new smoothness measures for new problems on hypergraphs.

We conduct experiments to show that our sparsely smooth models are beneficial to learning irrelevant and noisy data, and usually give similar or improved performances compared to non-sparse models. We compare predictive performance on benchmark categorical data with hyperedges being objects having a common categorical value. Experimental results can be found in Figure 2. The highlighted numbers are the highest AUCs, showing the highest performance, which means the most suitable models for the data.

Reference:

Canh Hao Nguyen and Hiroshi Mamitsuka, "Learning on Hypergraphs with Sparsity", *IEEE Transactions on Pattern Analysis and Machine Intelligence*, accepted (2020).

Dataset	n	m	Dense	Hyperedge Select.	Node Select.	Joint Select.
HayesRoth	132	15	0.587±0.044	0.600±0.071	0.758±0.076	0.746±0.067
Lenses	24	9	0.730±0.215	0.574±0.248	0.767±0.227	0.770±0.227
Congress	435	48	0.373±0.011	0.473±0.012	0.444±0.010	0.306±0.034
Spect	267	44	0.384±0.035	0.400±0.021	0.405±0.057	0.404±0.031
TicTacToe	958	27	0.468±0.009	0.476±0.009	0.481±0.019	0.476±0.009
Car	1728	21	0.692±0.043	0.462±0.026	0.748±0.043	0.740±0.044
Monks	124	17	0.469±0.008	0.437±0.023	0.528±0.029	0.504±0.004
Balance	625	20	0.831±0.013	0.955±0.010	0.916±0.014	0.629±0.044

Figure 2. Results of newly proposed sparsely smooth models on benchmark data.



HAKUBI RESEARCHERS' **A**CTIVITIES IN ICR

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





Program-Specific Assist Prof
DENIS ROMERO, Fabio
(Ph D)

Host Laboratory Laboratory of Advanced Solid State Chemistry

Host Professor SHIMAKAWA, Yuichi

Outline of Research

The wide range of electronic, magnetic, and transport properties exhibited by oxide materials has led to their widespread adoption as the basis of electronic devices and consequently contributed greatly to the exponential technological development over the past century. Continuing progress is fundamentally dependent on the discovery of new materials and the tunability of their fundamental properties. However, traditional synthetic methods are fundamentally unsuited to the preparation of a wide range of materials that could be imagined, and thus the development of new synthetic protocols is necessary to drive materials discovery forwards. My research focuses on the use of low-temperature topochemical methods and extreme conditions in order to prepare new materials with technologically useful properties for future devices.



ACTIVITIES OF
INTERNATIONAL **J**OINT
USAGE/**R**ESEARCH
CENTER

iJURC Cooperative Research Subjects 2020

(1 April 2020 ~ 31 March 2021)

STARTING-UP SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY iJURC)

Fabrication and Design of Chiral Plasmonic Nanostructures Based on Chemical Methods
NAKAGAWA, Makoto, Osaka Research Institute of Industrial Science and Technology
Host in iJURC KURATA, Hiroki

Study of Formation of Fine Periodic Structures Induced by Two Color Optical Pulses
NAGASHIMA, Takeshi, Faculty of Science and Engineering, Setsunan University
Host in iJURC HASHIDA, Masaki

Development of New Nano-structure Target for ISOL
OHNISHI, Tetsuya, SCRIT Team, Instrumentation Development Group, Nishina Center for Accelerator-Based Science, RIKEN
Host in iJURC WAKASUGI, Masanori

Study of Strange Structures of Short-lived Unstable Nuclei by Electron Scattering
SUDA, Toshimi, Electron Photon Science Laboratory, Tohoku University
Host in iJURC WAKASUGI, Masanori

Gas Sensing Properties Research of Transition-metal Oxides
GUO, Haichuan, Ningbo Institute of Industrial Technology (CNITECH) of the Chinese Academy of Sciences
Host in iJURC SHIMAKAWA, Yuichi I

Separation and Evaluation of Thiolate Protected Metal Clusters with Atomic Precision by Using LC/MS
NEGISHI, Yuichi, Department of Applied Chemistry, Tokyo University of Science
Host in iJURC TAKAYA, Hikaru I

Iron-catalyzed C-H Borylation
HAJRA, Alakananda, Department of Chemistry, Visva-Bharati University
Host in iJURC NAKAMURA, Masaharu I

Electrochemically Engineered Peptide Based Organic-Inorganic Nanohybrids for Electrocatalytic Conversion of Biomass into Value Added Chemicals
DAS, Apurba K., Department of Chemistry, Indian Institute of Technology Indore
Host in iJURC NAKAMURA, Masaharu I

Iron-catalyzed Enantioselective Carbometalation and Ring-opening Reactions of Oxabicycloalkenes and other Related Substrates and Mechanistic Consideration
ADAK, Laksmikanta, Department of Chemistry, Indian Institute of Engineering Science and Technology
Host in iJURC NAKAMURA, Masaharu I

Functionalization of Urushiol Coating Film Using Magnetic Particles
TACHIBANA, Yoichi, Kyoto Municipal Institute of Industrial Technology and Culture
Host in iJURC NAKAMURA, Masaharu

A Study on Statistical Machine Learning for Efficient Graph Structured Data Analysis
KARASUYAMA, Masayuki, Department of Computer Science, Nagoya Institute of Technology
Host in iJURC MAMITSUKA, Hiroshi I

Revealing Associations Between Giant Viruses and Eukaryotes in the Global Ocean Through Community Networks Inference and Mining
CHAFFRON, Samuel, Laboratoire des Sciences du Numérique de Nantes (LS2N), Centre National de la Recherche Scientifique (CNRS)
Host in iJURC ENDO, Hisashi I

Unveiling the Genomic Contents of Ecologically Important Marine Giant Viruses
DELMONT, Tom, Genoscope, Centre National de la Recherche Scientifique (CNRS)
Host in iJURC OGATA, Hiroyuki I

Development of Predictive Methods for Marine Microbial Communities Based on Remote Sensing Data
TOMII, Kentaro, Artificial Intelligence Research Center, The National Institute of Advanced Industrial Science and Technology
Host in iJURC OGATA, Hiroyuki

Control and Analysis of Complex Networks via Probabilistic Minimum Dominating Sets
NACHER, Jose C., Department of Information Science, Faculty of Science, Toho University
Host in iJURC AKUTSU, Tatsuya

Genomics and Transcriptomics of Giant Viruses
TAKEMURA, Masaharu, Faculty of Science, Tokyo University of Science
Host in iJURC OGATA, Hiroyuki

Whole Genome Analyses of Marine Bacterivorous Heterotrophic Nanoflagellates
KATAOKA, Takafumi, Faculty of Marine Science and Technology, Fukui Prefectural University
Host in iJURC ENDO, Hisashi

Comparative Genome Analysis of Parmales and Diatoms: Looking for the Ancestral Genomic Feature
SATO, Shinya, Faculty of Marine Science and Technology, Fukui Prefectural University
Host in iJURC OGATA, Hiroyuki

Exploration of Cycloaddition Properties of Guanidine Functionalized Anthracenes
DAVOR, Margetic, Division of Organic Chemistry and Biochemistry, Rudjer Boskovic Institute
Host in iJURC MURATA, Yasujiro I

Preparation of Dynamic Induced-helical Conformation in Block Copolymer and Investigation of Its Dominant Factor
HIRAI, Tomoyasu, Osaka Institute of Technology
Host in iJURC TAKENAKA, Mikihiro

I: International Joint Research

F: Female PI

Development of Kinetic Resolution for N-N Axial Chirality by Organocatalyst
YOSHIDA, Keisuke, Faculty of Pharmacy, Meijo University
Host in iJURC KAWABATA, Takeo

Molecular Understanding on the Structures and Dynamics of Ionic End-aggregation Polymers
VAO-SOONGNERN, Visit, School of Chemistry, Suranaree University of Technology
Host in iJURC WATANABE, Hiroshi I

Dynamics of Shear-induced Concentration Fluctuation in Polymer Solutions
ENDOH, Maya K., Department of Material Science and Chemical Engineering, Stony Brook University
Host in iJURC TAKENAKA, Mikihito I F

Identification of an Active Gibberellin Compound in the Basal Land Plant *Marchantia polymorpha*
KOHCHI, Takayuki, Graduate School of Biostudies, Kyoto University
Host in iJURC YAMAGUCHI, Shinjiro

Dynamic Viscoelasticity and Tensile Properties of Thermoplastic Elastomers
NORO, Atsushi, Department of Applied Chemistry, Nagoya University
Host in iJURC WATANABE, Hiroshi

Construction of Theoretical Guidelines for Designing Plasmonic Nanoalloys
IIDA, Kenji, Institute for Catalysis, Hokkaido University
Host in iJURC TERANISHI, Toshiharu

Study on Transportation of Metal Ions Through a Polymer Membrane Containing Ionic Liquid
MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education
Host in iJURC SOHRIN, Yoshiki

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY iJURC)

Unveil the Effect of Vibrational Strong Coupling on Molecular Reactivity
HIRAI, Kenji, Research Institute for Electronic Science, Hokkaido University
Host in iJURC KANEMITSU, Yoshihiko

X-Ray Structural Studies on Ligand Complexes of Maleylacetate Reductase
OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University
Host in iJURC FUJII, Tomomi

New Functionalities on Metal Surface with Controlling Laser Plasma Density
KUSABA, Mitsuhiro, Department of Electronics, Information and Communication Engineering, Faculty of Engineering, Osaka Sangyo University
Host in iJURC HASHIDA, Masaki

Small Molecule Activation Using Anionic Crypto-FLPs
STREUBEL, Rainer, Institute for Inorganic Chemistry, University of Bonn
Host in iJURC TOKITOH, Norihiro I

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 I

Development of Unsymmetrical π -Electron Systems of Heavier Main Group Elements and Elucidation of Their Property
IWAMOTO, Takeaki, Department of Chemistry, Tohoku University
Host in iJURC TOKITOH, Norihiro I

Optical Control of High-order Harmonic Generation from Solids
SATO, Shunsuke A., Max-Planck Institute for Structure and Dynamics of Matter/Center for Computational Sciences, University of Tsukuba
Host in iJURC KANEMITSU, Yoshihiko I

Study on the Stability of Novel Ternary Nanoparticles by Doping 3rd Elements
TATETSU, Yasutomi, Liberal Arts Education Center, Meio University
Host in iJURC TERANISHI, Toshiharu

Development of an Ultrashort Mid-infrared Light Source for Highly Efficient Extreme Nonlinear Optics in Solids
ISHII, Nobuhisa, National Institutes for Quantum and Radiological Science and Technology
Host in iJURC KANEMITSU, Yoshihiko

Magnon-phonon Excitation in Multiferroic Materials by Intense Terahertz Pulses
SATO, Takuya, Department of Physics, Tokyo Institute of Technology
Host in iJURC HIRORI, Hideki

Comprehensive Understanding and Modeling of the Termination Mechanism in Radical Polymerization
NAKAMURA, Yasuyuki, Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science
Host in iJURC YAMAGO, Shigeru

Development of Dinuclear Nickel Complexes Based on a Monoanionic Tridentate Pincer-type Ligand
YAMAGUCHI, Yoshitaka, Faculty of Engineering, Yokohama National University
Host in iJURC NAKAMURA, Masaharu

Creation of Effective Oxidation Scavenger for Efficient Perovskite-based Solar Cells
SASAMORI, Takahiro, Division of Chemistry, Faculty of Pure and Applied Sciences, University of Tsukuba
Host in iJURC WAKAMIYA, Atsushi

Integrating Omics Data and Module-based Network with Deep Learning to Develop Cancer Type Predictive Models
YANG, Jinn-Moon, Department of Biological Science and Technology, National Chiao Tung University /Institute of Bioinformatics & Systems Biology
Host in iJURC AKUTSU, Tatsuya I

Next-generation Bioinformatics Approaches for the Accurate Identification of Protease-specific Substrate Cleavage Sites
SONG, Jiangning, Biomedicine Discovery Institute, Monash University
Host in iJURC AKUTSU, Tatsuya I

Statistical Machine Learning Methods and Applications in Molecular Network Analysis

KAYANO, Mitsunori, Research Center for Global Agromedicine, Obihiro University of Agriculture and Veterinary Medicine
Host in iJURC MAMITSUKA, Hiroshi

Light Emission from Halide Perovskites and Related Materials
LIU, Ru-Shi, Department of Chemistry, National Taiwan University

Host in iJURC KANEMITSU, Yoshihiko I

Development of New Blue TADF Emitters with Horizontal Molecular Orientations

ZYSMAN-COLMAN, Eli, EaStCHEM School of Chemistry, Organic Semiconductor Centre, University of St Andrews

Host in iJURC KAJI, Hironori I

Coupling of Nanographenes and Curved π -Systems and Elucidation of Their Electronic and Optical Interactions

NARITA, Akimitsu, Organic and Carbon Nanomaterials Unit, Okinawa Institute of Science and Technology Graduate University (OIST)

Host in iJURC HIROSE, Takashi I

Development of Hole Transport Materials for Tin-perovskite and Device Characterization

SAEKI, Akinori, Department of Applied Chemistry, Graduate School of Engineering, Osaka University

Host in iJURC WAKAMIYA, Atsushi I

Development of π -Conjugated Nickel Complexes for High Performance n-Type Thermoelectric Materials

MURATA, Michihisa, Department of Applied Chemistry, Faculty of Engineering, Osaka Institute of Technology

Host in iJURC MURATA, Yasujiro

Synthesis of Novel Organic Functional Dye Bearing Heteroazulene Unit

KUROTOBI, Kei, Department of Liberal Arts (Natural Science and Mathematics), National Institute of Technology, Kurume College

Host in iJURC MURATA, Yasujiro

A Study of Reactive Intermediates in Macrocyclic Systems

ABE, Manabu, Department of Chemistry, Graduate School of Science, Hiroshima University

Host in iJURC YAMAGO, Shigeru

Observation of Orbital Hall Effect in Ferromagnet/Nonmagnet Bilayers

KIM, Sanghoon, Department of Physics, University of Ulsan

Host in iJURC ONO, Teruo I

High Frequency Response of Polymeric Liquids: Rheology and Dielectric Relaxation

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

Host in iJURC WATANABE, Hiroshi I

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

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

Host in iJURC SOHRIN, Yoshiki I

Revealing Exciton Quenching Mechanisms in Thermally Activated Delayed Fluorescent Devices

SAMUEL, Ifor D. W., Organic Semiconductor Centre, SUPA, School of Physics and Astronomy, University of St Andrews

Host in iJURC KAJI, Hironori I

Fabrication of Low Bandgap Semiconductor Films and Their Light Induced Interfacial Charge Transfer and Charge Transport Dynamics

TACHIBANA, Yasuhiro, School of Engineering, RMIT University

Host in iJURC TERANISHI, Toshiharu I

Visualization of Sulfur Distribution in Polymer Thin Films Using GISAXS-CT

FUJIWARA, Akihiko, Kwansai Gakuin University

Host in iJURC TAKENAKA, Mikihito

Origin Analysis of Atmospheric Aerosol of Mountainous Areas by Trace Metal Analysis

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

Host in iJURC SOHRIN, Yoshiki

Analysis of Membrane Structure and Properties of Partially Fluorinated Amphiphilic Molecules

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

Host in iJURC HASEGAWA, Takeshi

Exploration of Hierarchical Dynamics of Amorphous Polymers by Broadband Dielectric Spectroscopy

URAKAWA, Osamu, Department of Macromolecular Science, Osaka University

Host in iJURC MATSUMIYA, Yumi

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

Dielectric Relaxation of Type-A Rouse Chain under End-adsorption/desorption Equilibrium: Effect of Motional Coupling

KWON, Youngdon, School of Chemical Engineering, Sungkyunkwan University

Host in iJURC MATSUMIYA, Yumi I

Role of PX-PH-type Phospholipase Ds in Plant Intracellular Membrane Traffic

OHASHI, Yohei, MRC Laboratory of Molecular Biology

Host in iJURC AOYAMA, Takashi I

Application of Artificial Viral Capsid to Intracellular Delivery

MATSUURA, Kazunori, Department of Chemistry and Biotechnology, Tottori University

Host in iJURC FUTAKI, Shiroh

Novel Strategy for Intracellular Delivery of Nanomedicines

PUJALS, Silvia, Nanoscopy for Nanomedicine Group, Institute for Bioengineering of Catalonia (IBEC)

Host in iJURC FUTAKI, Shiroh I F

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 I F

Formation of Supramolecular Complexes Through a Host-guest Interaction Between Cycloparaphenylene and Azacorannulenes

ITO, Shingo, Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University (NTU)

Host in iJURC YAMAGO, Shigeru I

Interdisciplinary Approach to Nanostructured Materials for Applications

BUCHER, Jean-Pierre, Institut de Physique et Chimie des Matériaux (IPCMS), Université de Strasbourg

Host in iJURC TERANISHI, Toshiharu I

Relationship between Chain Orientation, Amount of Defects, and Toughness of Glassy Polystyrene Materials

CHEN, Quan, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences (CAS)

Host in iJURC MATSUMIYA, Yumi I

Fabrication of Thin Films and Structural Characterization of Self-Assembled Lanthanoid Complexes

MIEDA, Eiko, Graduate School of Science Molecular Materials Science Course, Osaka City University

Host in iJURC HASEGAWA, Takeshi F

Study on the Regulatory Network of Plant Epidermal Cell Differentiation

TOMINAGA, Rumi, Graduate School of Integrated Sciences for Life, Hiroshima University

Host in iJURC AOYAMA, Takashi F

Immune-stimulatory Nano-assemblies

YAMASAKI, Sho, Research Institute for Microbial Disease, Osaka University

Host in iJURC UESUGI, Motonari

Analysis of Phase Equilibrium and Molecular Dynamics in Mixture of Nematic Liquid Crystal and Solvent

SHIMADA, Ryoko, Department of Mathematical and Physical Sciences, Japan Women's University

Host in iJURC WATANABE, Hiroshi F

Functional Analysis of the CYP711A Family in Strigolactone Biosynthesis of Rice

IZAWA, Takeshi, Graduate School of Agricultural and Life Sciences, The University of Tokyo

Host in iJURC MASHIGUCHI, Kiyoshi

Self-assembling Molecules for Improvement of Cardiomyocyte Engraftment

SHIBA, Yuji, School of Medicine, Shinshu University

Host in iJURC UESUGI, Motonari

Giant Exchange Reaction from H to D Terminating on Nanocrystalline Silicon Surface and Their Use

MATSUMOTO, Takahiro, Graduate School of Design and Architecture Industrial Innovation Design, Nagoya City University

Host in iJURC KANEMITSU, Yoshihiko

Solid Phase Extraction of Metal Ion by Solvent Impregnated Resin Using Surfactant

KURAHASHI, Kensuke, Environmental and Materials Chemistry Course, Osaka Prefecture University College of Technology

Host in iJURC SOHRIN, Yoshiki

Studies on Aromaticity of Cyclic Paraphenylenes with Möbius Topology

FUJITSUKA, Mamoru, The Institute of Scientific and Industrial Research, Osaka University

Host in iJURC YAMAGO, Shigeru

Study on Electronic and Magnetic Behavior of Perpendicularly Magnetized Cobalt Ferrite Films

TANAKA, Masaaki, Department of Physical Science and Engineering, Nagoya Institute of Technology

Host in iJURC ONO, Teruo

Study of the Generation and Sustainment of High Energy Density Plasmas due to the Interaction between High Power Laser and Structured Medium

KISHIMOTO, Yasuaki, Graduate School of Energy Science, Kyoto University

Host in iJURC INOUE, Shunsuke

Functional Analysis of Membrane Lipids on Environmental Stress Tolerance in Acetic Acid Bacteria

TOYOTAKE, Yosuke, Department of Biotechnology, College of Life Sciences, Ritsumeikan University

Host in iJURC OGAWA, Takuya

Study on Water Freezing with Cellulose and Their Anti-icing Control by Surface Modification

SAKAKIBARA, Keita, National Institute of Advanced Industrial Science and Technology

Host in iJURC TSUJII, Yoshinobu

Asymmetric Umpolung C–C Bond Formation via Expression of Dynamic Chirality

MORIYAMA, Katsuhiko, Graduate School of Science, Chiba University

Host in iJURC KAWABATA, Takeo

Studies on Enantioselective Total Syntheses of Marine Natural Product Bohemamines and Their Derivatives

YOSHIMURA, Tomoyuki, Division of Pharmaceutical Sciences, Graduate School of Medical Science, Kanazawa University

Host in iJURC KAWABATA, Takeo

Development of Efficient Conversion Method of Woody Biomass, Renewable Biological Resources, to Advanced Chemical Materials

HATANO, Osamu, Nara Medical University

Host in iJURC NAKAMURA, Masaharu

EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Molecular Mechanisms for the Inactivation of a Growth Hormone in Rice

HE, Zuhua, Institute of Plant Physiology and Ecology, CAS Center for Excellence in Molecular Plant Sciences, Chinese Academy of Sciences

Host in iJURC YAMAGUCHI, Shinjiro I

Well-defined AIE-based Polymer Brush for the Application of the Electrochemical Luminescence Biosensors

MA, Ying, Chemistry and Chemical Engineering, South China University of Technology

Host in iJURC OHNO, Kohji I

Role of Phosphoinositide Signaling in Pollen Development

ZHONG, Sheng, School of Life Sciences, Peking University

Host in iJURC AOYAMA, Takashi I F

Proteomic Approach to Discovering Specific Inhibitors for Bile-acid Interacting Enzymes

LEI, Xiaoguang, College of Chemistry and Molecular Engineering, Peking University

Host in iJURC UESUGI, Motonari I

Transfer of Redox Sensitive Elements (Fe, Mn, Zn) Across the Sediment-water Interface in a Hypoxia Area Near the East Chia Sea

CAI, Pinghe, Department of Marine Chemistry and Geochemistry, Xiamen University

Host in iJURC SOHRIN, Yoshiki I

- Structural and Functional Analysis of Curvature-inducing Peptides and Application
ULRICH, Anne S., Institute of Organic Chemistry (IOC) and Institute of Biological Interfaces (IBG-2), Karlsruhe Institute of Technology (KIT)
Host in iJURC FUTAKI, Shiroh I F
- Site-selective Protein Acetylation by a Small Molecule
ZHOU, Lu, School of Pharmacy, Fudan University
Host in iJURC UESUGI, Motonari I
- Modulation of Ferrimagnetic Spin Waves by Electric Field
KIM, Kab-Jin, Department of Physics, Korea Advanced Institute of Science and Technology
Host in iJURC ONO, Teruo I
- Development of Highly Efficient and Stable Blue Organic Light Emitting Diodes Using Thermally Activated Delayed Fluorescent Materials with Ultrafast Reverse Intersystem Crossing
DUAN, Lian, Department of Chemistry, Tsinghua University
Host in iJURC KAJI, Hironori I
- Fabrication of Nanotopographical Polymer Surfaces for Bactericidal Properties-II
ENDO, Maya K., Department of Material Science and Chemical Engineering, Stony Brook University
Host in iJURC TAKENAKA, Mikihito I F
- Synthesis of Polyether Nanocomposite Solid Polymer Electrolytes for Lithium Ion Batteries
FERRIER, Robert C., Chemical Engineering and Materials Science, Michigan State University
Host in iJURC OHNO, Kohji I
- Structural and Functional Analysis of the Surface Glycolipids of Outer Membrane Vesicles Released by Bacteria
CORSARO, Maria Michela, Department of Chemical Sciences, University of Naples Federico II
Host in iJURC KURIHARA, Tatsuo I F
- Molecular Mechanisms Governing Gene Expression Regulation in Plant Plasticity
RUBIO, Vicente, Plant Molecular Genetics Department, National Center of Biotechnology (CNB-CSIC)
Host in iJURC TSUGE, Tomohiko I
- Research of Multi-qubit Diamond Quantum Processors
DOHERTY, Marcus W., Research School of Physics and Engineering, Australian National University
Host in iJURC MIZUOCHI, Norikazu I
- Research Toward Stable NV Centers at Shallow Region in Diamond
BALASUBRAMANIAN, Gopalakrishnan, Max-Planck Institute for Biophysical Chemistry
Host in iJURC MIZUOCHI, Norikazu I
- Advanced Iodine – Mediated Stereoselective Flow Electrochemistry
WIRTH, Thomas, School of Chemistry, Cardiff University
Host in iJURC KAWABATA, Takeo I
- Cation- π Interaction in Enolate Chemistry
CLAYDEN, Jonathan, School of Chemistry, University of Bristol
Host in iJURC KAWABATA, Takeo I
- Search for Four-wave-mixing in the Vacuum–Unveiling Dark Components in the Universe –
HOMMA, Kensuke, Physics, Hiroshima University
Host in iJURC INOUE, Shunsuke I
- Fine Synthesis of Polymer Brush on Ferromagnetic Nano-platelet for Magnetophotonic LC
UCHIDA, Yoshiaki, Graduate School of Engineering Science, Osaka University
Host in iJURC OHNO, Kohji
- Functional Analysis of Non-canonical Strigolactones as Plant Hormones and Root-derived Signals
SETO, Yoshiya, School of Agriculture, Meiji University
Host in iJURC YAMAGUCHI, Shinjiro
- Analysis of the Physiological Functions of Extracellular Vesicles Produced by Intestinal Bacteria and Fermented Food-derived Bacteria and Their Application
KURATA, Atsushi, Faculty of Agriculture, Kindai University
Host in iJURC KURIHARA, Tatsuo
- Observation of Spin Wave Propagation in Polycrystalline YIG Thin Films Prepared by Coprecipitation Method
YAMADA, Keisuke, Materials Chemistry Course, Department of Chemistry and Biomolecular Science, Graduate School of Engineering, Gifu University
Host in iJURC ONO, Teruo
- Control of Malignant Behavior of Colorectal Cancer by Antitumoral Cell Penetrating Peptide (CPP)
OHASHI, Wakana, Department of Pharmaceutical Sciences, Keio University
Host in iJURC FUTAKI, Shiroh F
- Anomalous Hall Effect of Ultrathin Pt Films Grown on Magnetic Oxide
NAGAHAMA, Taro, Solid State Chemistry Laboratory, Faculty of Engineering, Hokkaido University
Host in iJURC ONO, Teruo
- Synthesis and Study of Oxides with Unusually High-valent Cation
SAITO, Takashi, High Energy Accelerator Research Organization (KEK)
Host in iJURC SHIMAKAWA, Yuichi
- Prediction of Charge Transport Mobilities of Organic p-Type Semiconductors based on Multiscale Simulation
KIDO, Junji, Department of Organic Device Engineering, Yamagata University
Host in iJURC KAJI, Hironori
- Development of Novel π -Conjugated Polymers by DArP and Their Application to Organic Photovoltaics
OSAKA, Itaru, Graduate School of Engineering, Hiroshima University
Host in iJURC WAKIOKA, Masayuki
- Spin and Valence Electron Dependent Au₂₅ Ferromagnetic Single-electron Transistor
MAJIMA, Yutaka, Materials and Structures Laboratory, Tokyo Institute of Technology
Host in iJURC TERANISHI, Toshiharu
- Manufacture of Nano-scale Shallow NV Centers in Diamond
TOKUDA, Norio, Nanomaterials Research Institute, Kanazawa University
Host in iJURC MIZUOCHI, Norikazu
- Electrical Control and Detection of Spin of NV Center
MAKINO, Toshiharu, National Institute of Advanced Industrial Science and Technology (AIST)
Host in iJURC MIZUOCHI, Norikazu

Theoretical Study on Chemoselective Acylation Catalyzed by 4-Pyrrolidinopyridine Derivatives
YAMANAKA, Masahiro, Department of Chemistry, Rikkyo University
Host in iJURC KAWABATA, Takeo

SUBJECTS FOCUSING OF JOINT USAGE OF iJURC/ICR FACILITIES

Study on the Mechanism of the Crystal Structural Evolution of Polydimethylsiloxane
LI, Liangbin, National Synchrotron Radiation Laboratory, University of Science and Technology of China
Host in iJURC TOSAKA, Masatoshi [I]

High-pressure Synthesis of Potential Multiferroic Oxides
JI, Kunlang, Centre for Science at Extreme Conditions and School of Chemistry, University of Edinburgh
Host in iJURC SHIMAKAWA, Yuichi [I]

Micro- and Nano-structural Characterization by Advanced Transmission Electron Microscopy of Novel Functional Materials for Battery Development
CHAIRUANGSR, Torranin, Industrial Chemistry, Chiang Mai University
Host in iJURC KURATA, Hiroki [I]

Electron Energy Loss Spectroscopy Analysis of Hexagonal Multilayer Graphene
WEN, Cheng-Yen, Department of Materials Science and Engineering, National Taiwan University
Host in iJURC KURATA, Hiroki [I]

Electronic Excitations in Charge-density-wave Systems
CHU, Ming-Wen, Center for Condensed Matter Sciences, National Taiwan University
Host in iJURC KURATA, Hiroki [I]

Synthesis and Characterization of Novel Organoselenium and -tellurium Compounds
MINOURA, Mao, Department of Chemistry, College of Science, Rikkyo University
Host in iJURC TOKITOH, Norihiro [I]

Elucidation of the Fluorous Interactions in the Crystal Structures of Fluorine-containing Conjugated Molecules by the Single-crystal X-ray Structural Analysis
AGOU, Tomohiro, Department of Materials Science and Engineering, College of Engineering, Ibaraki University
Host in iJURC TOKITOH, Norihiro

Synthesis and Structural Characterization of Low-valent Species of Heavier Group 14 Elements
MATSUO, Tsukasa, Faculty of Science and Engineering, Kindai University
Host in iJURC TOKITOH, Norihiro

Development of Functional Group Analysis on the Surface of Carbon Materials Using DNP-NMR
GOTOH, Kazuma, Department of Chemistry, Faculty of Science, Okayama University
Host in iJURC KAJI, Hironori

Theoretical Design of Planar Silicene Nanoribbons and Search for New Operating Principles
TAKAHASHI, Masae, Graduate School of Agricultural Science, Tohoku University
Host in iJURC TOKITOH, Norihiro [F]

High Accuracy Measurement of Hydrogen and Helium Behavior in Plasma Facing Materials for Nuclear Fusion Devices
MIYAMOTO, Mitsutaka, Interdisciplinary Faculty of Science and Engineering, Shimane University
Host in iJURC KURATA, Hiroki

Synthesis and Structures of Cationic Aromatics Bearing Thiopyrylium Units
NAGAHORA, Noriyoshi, Department of Chemistry, Faculty of Science, Fukuoka University
Host in iJURC TOKITOH, Norihiro

Analysis of Chemical Properties and Origins of Organic Matter in Lakes and Soils Using FT-ICR-MS
FUSE, Yasuro, Faculty of Molecular Chemistry and Engineering, Kyoto Institute of Technology
Host in iJURC NAKAMURA, Masaharu

STEM-EELS Analysis of Bound Excitons at Defects in Two-dimensional Materials
SAITO, Hikaru, Interdisciplinary Graduate School of Engineering Sciences, Kyushu University
Host in iJURC KURATA, Hiroki

SUBJECTS ENCOURAGING JOINT PROGRAM

Determine the Three-dimensional Structure of ¹³C Labeled α -Synuclein(61-95) in the Langmuir-Blodgett Film and Supported Phospholipids Bilayers by p-MAIRS FT-IR
WANG, Chengshan, Chemistry, Middle Tennessee State University
Host in iJURC HASEGAWA, Takeshi [I]

Hydrophilic Dendrimers as Additive for Polyvinylidene difluoride Based Membranes
SEMSARILAR, Mona, Institut Europeen des Membranes (IEM), CNRS
Host in iJURC YAMAGO, Shigeru [I]

Resolving Percolation Dynamics Responsible for Mechanical Reinforcement in Polymer Nanocomposites Under Uniaxial Stretching
KOGA, Tadanori, Department of Material Science and Chemical Engineering, Stony Brook University
Host in iJURC TAKENAKA, Mikihito [I]

The 16th International Workshop for East Asian Young Rheologists
INOUE, Tadashi, Department of Macromolecular Science, Osaka University
Host in iJURC MATSUMIYA, Yumi [I]

iJURC Publications (Selected Examples)

(until 31 May 2020)

Reversible Isomerizations between 1,4-Digermabenzenes and 1,4-Digerma-Dewar-benzenes: Air-stable Activators for Small Molecules

Sugahara, T.; Guo, J.-D.; Hashizume, D.; Sasamori, T.; Tokitoh, N., *J. Am. Chem. Soc.*, **141**, 2263-2267 (2019).

Abstract

The first examples of stable, crystalline, and air-sensitive 1,4-digermabenzenes were isolated. These species photochemically isomerize into the corresponding air-stable digerma-Dewar-benzenes. More importantly, alkyl-substituted Dewar-type-1,4-digermabenzenes can be considered as reversible "air-stable activators" for small molecules such as dihydrogen, carbon dioxide, and acetylene at room temperature. The regeneration of these activators can be accomplished via a thermal retro-isomerization that affords the corresponding 1,4-digermabenzenes.

H₂O/Olefinic- π Interaction inside a Carbon Nanocage

Hashikawa, Y.; Murata, Y., *J. Am. Chem. Soc.*, **141**, 12928-12938 (2019).

Abstract

The H₂O/CH₂=CH₂-type hydrogen-bonding (H-bonding) model was experimentally constructed using a water complex of an open-cage C₆₀ derivative, in which an olefinic double bond and a single molecule of H₂O are geometrically confined. To investigate OH/ π -type H-bonding, that is, H₂O \cdots (C=C) interaction, we performed ¹H NMR spectroscopic studies that demonstrated the monotonic downfield shift of the proton signal corresponding to H₂O with remarkable rotational perturbation by lowering the temperature. From the temperature dependence of the angular momentum correlation time (τ_j), the interaction energy was quantitatively estimated to be ca. 0.3 kcal/mol. The computational studies were thoroughly conducted to clarify its inherent nature. As a consequence, the orientation of H₂O was found to play a prominent role in varying the bonding strength as well as contribution from the electrostatic attraction and orbital-orbital interaction significantly driven by the favorable orbital overlap identified as $\pi(\text{C}=\text{C}) \rightarrow \sigma^*(\text{OH})$ interaction.

Bulk Dzyaloshinskii-Moriya Interaction in Amorphous Ferrimagnetic Alloys

Kim, D.-H.; Haruta, M.; Ko, H.-W.; Go, G.; Park, H.-J.; Nishimura, T.; Kim, D.-Y.; Okuno, T.; Hirata, Y.; Futakawa, Y.; Yoshikawa, H.; Ham, W.; Kim, S.; Kurata, H.; Tsukamoto, A.; Shiota, Y.; Moriyama, T.; Choe, S.-B.; Lee, K.-J.; Ono, T., *Nat. Mater.*, **18**, 685-690 (2019).

Abstract

Symmetry breaking is a fundamental concept that prevails in many branches of physics. In magnetic materials, broken inversion symmetry induces the Dzyaloshinskii-Moriya interaction (DMI), which results in fascinating physical behaviours with the potential for application in future spintronic devices. Here, we report the observation of a bulk DMI in GdFeCo amorphous ferrimagnets. The DMI is found to increase linearly with an increasing thickness of the ferrimagnetic layer, which is a clear signature of the bulk nature of DMI. We also found that the DMI is independent of the interface between the heavy metal and ferrimagnetic layer. This bulk DMI is attributed to an asymmetric distribution of the elemental content in the GdFeCo layer, with spatial inversion symmetry broken throughout the layer. We expect that our experimental identification of a bulk DMI will open up additional possibilities to exploit this interaction in a wide range of materials.

Dielectric Relaxation of Type-A Chains Undergoing Head-to-Tail Association/Dissociation: Difference from Head-to-Head Case and Correlation with Viscoelastic Relaxation

Kwon, Y.; Matsumiya, Y.; Watanabe, H., *Macromolecules*, **52**, 8484-8502 (2019).

Abstract

Dielectric relaxation of type-A chains reflects global motion of the chains but is also affected by relative alignment of the dipoles along the chain backbone, namely, by the dipole inversion. Head-to-head association of type-A unimers gives a symmetrically dipole-inverted dimer, and the association/dissociation equilibrium of these unimers and dimer results in motional coupling of these chains, thereby affecting the dielectric behavior. In fact, for this head-to-head case, eigenmode analysis has been reported in the literature to reveal that motional coupling results in moderate retardation and acceleration of the dielectric relaxation of the unimer and dimer obeying the reptation dynamics. In contrast, the coupling has no effect on the dielectric relaxation of the Rouse unimer and dimer, namely, the effect of motional coupling on the dielectric relaxation changes with the type of chain dynamics. This effect was not clarified for head-to-tail associating unimers and their dimer having no dipole inversion. Thus, for completeness, this study makes the eigenmode analysis of the dielectric relaxation for this case of head-to-tail reaction. For the unimer and dimer obeying either Rouse or reptation dynamics, the analysis indicates that the retardation and acceleration of the dielectric relaxation of the unimer and dimer are much more significant for the head-to-tail case than for the head-to-head case irrespective of the chain dynamics, and that the dielectric relaxation function for the former case exactly coincides with the viscoelastic relaxation function if the unimer and dimer obey the reptation dynamics. This result suggests an interesting method of resolving some detail of the chain dynamics under the reaction through comparison of dielectric and viscoelastic responses of the associative type-A chains.

Probabilistic Controllability Approach to Metabolic Fluxes in Normal and Cancer Tissues

Schwartz, J.-M.; Otokuni, H.; Akutsu, T.; Nacher, J. C., *Nat. Commun.*, **10**, 2725 (2019).

<https://doi.org/10.1038/s41467-019-10616-z>

Abstract

Recent research has shown that many types of cancers take control of specific metabolic processes. We compiled metabolic networks corresponding to four healthy and cancer tissues, and analysed the healthy-cancer transition from the metabolic flux change perspective. We used a Probabilistic Minimum Dominating Set (PMDS) model, which identifies a minimum set of nodes that act as driver nodes and control the entire network. The combination of control theory with flux correlation analysis shows that flux correlations substantially increase in cancer states of breast, kidney and urothelial tissues, but not in lung. No change in the network topology between healthy and cancer networks was observed, but PMDS analysis shows that cancer states require fewer controllers than their corresponding healthy states. These results indicate that cancer metabolism is characterised by more streamlined flux distributions, which may be focused towards a reduced set of objectives and controlled by fewer regulatory elements.



VISITING PROFESSORS'
ACTIVITIES IN ICR



Vis Prof
TOKUDA, Norio
(Ph D)

Laboratory of Inorganic Photonics Materials
Professor, Nanomaterials Research Institute,
Kanazawa University
(Kakuma, Kanazawa, Ishikawa 920-1192)

Lecture at ICR
High Quality Diamond CVD Synthesis for
Quantum Sensor



Vis Prof
YAMADA, Hiroko
(D Sc)

Laboratory of Chemistry for Functionalized
Surfaces

Professor, Division of Materials Science,
Graduate School of Science and Technology,
Nara Institute of Science and Technology
(8916-5 Takayama-cho, Ikoma, Nara 630-
0192)

Lecture at ICR
Synthesis of Functional Materials Using the
Precursor Approach



Vis Prof
MUTO, Shunsuke
(D Eng)

Laboratory of Electron Microscopy and
Crystal Chemistry

Professor, Institute of Materials and Sys-
tems for Sustainability, Nagoya University
(Furo-cho, Chikusa-ku, Nagoya 464-8601)

Lecture at ICR
Nano Level Analysis and Visuarization of
Functional Materials Using Electron Nao-
Spectroscopic Methods



Vis Prof
OKADA, Mariko
(D Agr)

Laboratory of Bio-knowledge Engineering

Professor, Institute for Protein Research,
Osaka University
(3-2 Yamadaoka, Suita-shi, Osaka 565-0871)

Lecture at ICR
Understanding Life Phenomena by Systems
Biology and Machine Learning



Vis Assoc Prof
SOHTOME, Yoshihiro
(D Pharm Sc)

Laboratory of Synthetic Organic Chemistry
Senior Research Scientist, Synthetic Organic
Chemistry Laboratory, RIKEN
(2-1 Hirosawa, Wako, Saitama 351-0198)

Lecture at ICR
Dynamic Catalysis: Toward Symbiosis
between Molecular Catalysts and Enzymes



Vis Assoc Prof
HAYASHI, Gosuke
(D Sc)

Laboratory of Biofunctional Design-Chemistry

Associate Professor, Department of Bio-
molecular Engineering, Graduate School of
Engineering, Nagoya University
(Furo-cho, Chikusa-ku, Nagoya 464-8603)

Lecture at ICR
Design and Synthesis of Histone Proteins
for Epigenetic Analysis



Vis Assoc Prof
YASHIRO, Wataru
(D Eng)

Laboratory of Polymer Materials Science
Associate Professor, Institute of Multidisci-
plinary Research for Advanced Materials,
Tohoku University
(2-1-1 Katahira, Aoba-ku, Sendai 980-8577)

Lecture at ICR
High-speed Multi-beam X-ray Imaging
Using a Lens Coupling Detector System



Vis Assoc Prof
SUNADA, Yusuke
(D Sc)

Laboratory of Synthetic Organotransformation

Associate Professor, Institute of Industrial
Science, The University of Tokyo
(4-6-1 Komaba, Meguro-ku, Tokyo 153-
8505)

Lecture at ICR
1. Organometallic Complex Chemistry
2. Organometallic Complex and Cluster
Chemistry



Prof Em KANEHISA, Minoru (D Sc)
Appointed as Res (pt) at ICR,
1 April 2012–31 March 2021



PERSONAL

Retirement

Professor KAWABATA, Takeo
Division of Synthetic Chemistry
– Synthetic Organic Chemistry –



On March 31st 2021, Dr. Takeo Kawabata retired from Kyoto University after 32 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Kawabata was born in Osaka Prefecture on June 12, 1955. He graduated from Faculty of Pharmaceutical Sciences, Kyoto University in 1978, and entered the graduate school. He received the doctoral degree under the direction of Professor Eiich Fujita and Professor Kaoru Fuji in 1983. He studied total synthesis of natural products as a post-doctoral fellow at Indiana University with Professor Paul A. Grieco in 1983–1985. He moved to Sagami Chemical Research Center in 1985, and studied enolate chemistry and asymmetric synthesis of β -lactams with Professor Tamejiro Hiyama and Professor Shiro Terashima. He was appointed an Assistant Professor at ICR in 1989, promoted as Associate Professor in 1998, and Professor in 2004.

Throughout his academic career, Dr. Kawabata's research has been focused on "dynamic chirality" and "dynamic molecular recognition". He proposed dynamic chirality in enolate structure in 1991, and proved that enolates can exist as a chiral form in a limited time scale based on restricted bond rotation around C-C, C-N, and C-O bonds. Since enolates are representative synthetic intermediates, the discovery of dynamic chirality in enolate structure brought a conceptually novel strategy for asymmetric synthesis. The concept of "memory of chirality" was generally recognized, and widely applied in various types of asymmetric syntheses. As an extreme example, asymmetric reactions took place in up to 99% enantiomeric excess via a short-lived chiral enolate intermediate based on the restricted C-O bond rotation, whose half-life of racemization was assumed to be ~ 1 sec at -78 °C. The methods were also applied to industrial production of an anti-tumor drug, veripalib (AbbVie (former Abbott)).

He developed an organocatalyst for asymmetric acylation of alcohols in 1997. The salient feature of the catalyst is conformational change triggered by binding with the reagent (anhydride) via an "induced fit process". In 2007, he developed a catalyst for site-selective acylation of glucose derivatives. The catalyst enables to deliver acyl groups into a secondary hydroxy group at C(4) of the glucose core even in the presence of intrinsically more reactive primary hydroxy group at C(6). The molecular recognition process is highly functional group-tolerant, and the acylation takes places with the desired site-selectivity in the presence of various hydrogen bond donors and acceptors. Recognition of the transition state structure (dynamic molecular recognition) seems to be the key to achieve the catalyst-controlled site-selectivity.

The outstanding properties of the catalyst realized extremely short-step total syntheses of natural glycosides. An anti-viral natural glycoside, strictinin (MW 634), has been synthesized from naturally abundant glucose in only 5 steps. The overall synthetic steps were less than half compared with those (11~13 steps) in the previous reports because the the present synthetic route can eliminate the use of protective groups for glucose. Accordingly, he proposed a non-conventional retro-synthetic analysis for total synthesis of natural products based on site-selective and sequential functionalization of unprotected glucose. The strategy was further applied to total syntheses of middle-weight natural glycosides such as tellimagrandin II (MW 938), pterocarinin C (MW 938), cercidinin A (MW 938), punicafolin (MW 938), macaranganin (MW 938), and coriariin A (MW 1874) in only 6 or 7 overall steps from glucose.

He then applied the catalytic strategy to remote asymmetric induction, and found that the related catalysts were quite useful in asymmetric desymmetrization of long chain linear diols by asymmetric acylation as well as asymmetric silylation. Asymmetric desymmetrization of bisphenol derivatives by catalytic bromination was also performed in a highly enantioselective manner. Finally, the strategy for remote asymmetric acylation was successfully applied to asymmetric synthesis of rotaxanes. Highly enantioselective synthesis of chiral mechanically interlocked molecules has been a long-standing dream in organic synthesis. Preparation of an enantiopure rotaxane was achieved by kinetic resolution of the racemate via remote asymmetric acylation promoted by the catalyst.

His educational contribution to Kyoto University is also noteworthy. He has supervised 82 graduate students (40 Ph. D. degrees and 42 Master degrees) and 8 undergraduate students and sent them out to academia and industry.

For his achievements, he was awarded the Pharmaceutical Society of Japan Award for Young Scientists from the Pharmaceutical Society of Japan in 1996, Molecular Chirality Award from Molecular Chirality Research Organization in 2012, the Pharmaceutical Society of Japan Award from the Pharmaceutical Society of Japan in 2017, and the Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology in 2018.

Dr. Kawabata's contribution to Kyoto University and ICR through his scientific research and education is highly appreciated. His sincere attitude toward science will remain in the memory of the people knowing him for a long time in the future.

Awards

OSHIRO, Taku



Oral Presentation Award

The 24th Symposium on The Society of Silicon Chemistry JAPAN

“Synthesis of 2-Germaazulene”

The Society of Silicon Chemistry JAPAN

6 November 2020

HIROSE, Takashi



Thieme Chemistry Journals Award 2020

Thieme Chemistry

“Breaking Up Kekulene, Resulting in π -Expanded Helicene”

The Editorial Board of SYNTHESIS, SYNLETT, and SYNFACTS

14 January 2020

The Japanese Photochemistry Association (JPA) Award for Young Scientist 2020

“Development of Highly Efficient Photophysical and Photoresponsive Functions Based on Rational Designs of π -Conjugated Compounds”

The Japanese Photochemistry Association

10 September 2020

UEDA, Yoshihiro



The Pharmaceutical Society of Japan Award for Young Scientists

“Development of Site-selective Acylation of Polyols and C-H Amination”

The Pharmaceutical Society of Japan

25 March 2020

NINOMIYA, Ryo



The Best Oral Presentation Award

The 46th Symposium on Progress in Organic Reactions and Syntheses

“Asymmetric Desymmetrization of σ -Symmetric Diarylmethylamines by Organocatalytic Aromatic Bromination”

The Pharmaceutical Society of Japan

10 November 2020

HASHIMOTO, Hisashi



The Best Oral Presentation Award

The 70th Annual Meeting of the Pharmaceutical Society of Japan Kansai Branch

“Organocatalytic Distance-selective Silylation of Aminoalcohols”

The Pharmaceutical Society of Japan

10 October 2020

HERBSCHLEB, Ernst David



The Best Oral Presentation Award

33rd Diamond Symposium

“Long Coherence Times and High Magnetic Sensitivity with Nitrogen-vacancy Centers in Phosphorus-doped Diamond”

Japan New Diamond Forum

19 May 2020

SO, Frederick Tzekit



Short Presentation Award

“A Simple Deaggregation Method Producing Single-digit Detonation Nanodiamonds”

The 3rd International Forum on Quantum Metrology and Sensing

24 December 2020

SHIOTA, Yoichi



ICR Award for Young Scientists

“Tunable Magnon-Magnon Coupling Mediated by Dynamic Dipolar Interaction in Synthetic Antiferromagnets”

Institute for Chemical Research, Kyoto University

11 December 2020

ISHIBASHI, Mio



ICR Award for Graduate Students

“Switchable Giant Nonreciprocal Frequency Shift of Propagating Spin Waves in Synthetic Antiferromagnets”

Institute for Chemical Research, Kyoto University

11 December 2020

FUTAKI, Shiroh



2019 Highly Cited Review Award for CPB

“Current Understanding of Direct Translocation of Arginine-rich Cell-penetrating Peptides and Its Internalization Mechanisms”

The Pharmaceutical Society of Japan

18 February 2020

The Pharmaceutical Society of Japan Award

“Functional Peptides that Target Biomembranes: Design and Modes of Action”

The Pharmaceutical Society of Japan

25 March 2020

ARAFILES, Jan Vincent V.



Excellent Stone Award

The 57th Japanese Peptide Symposium

“Extracellular Thiol-disulfide Exchange Reaction Produces Potent Macropinosytosis-inducing Peptide Analogs”

The Japanese Peptide Society

11 November 2020

SAKAMOTO, Kentarou



Good Stone Award

The 57th Japanese Peptide Symposium

“Artificial Viral Capsid to Deliver Biomacromolecules into Cytosol”

The Japanese Peptide Society

11 November 2020

YOSHIDA, Atsuhiko



The Best Oral Presentation Award

The 70th Annual Meeting of the Kansai Branch of the Pharmaceutical Society of Japan

“Mechanism of RNA Methylation via G-quadruplex Structures”

The Kansai Branch of the Pharmaceutical Society of Japan

10 October 2020

ZHENG, Linjie



ICR Award for Young Scientists

“Distinct Basin-scale-distributions of Aluminum, Manganese, Cobalt, and Lead in the North Pacific Ocean”

Institute for Chemical Research, Kyoto University

11 December 2020

TSUJISAKA, Makoto



Oceanography Encouragement Prize (U30)

“Development of Stable Isotope Ratio Analysis for Molybdenum and Tungsten in Sediments and Reconstruction of Paleoenvironment in the Japan Sea”

Research Institute for Oceanography Foundation

14 November 2020

HASEGAWA, Takeshi



Academic Prize of the Japan Society of Analytical Chemistry

The 69th Annual Meeting of the Japan Society of Analytical Chemistry

“Development and Practicalization of Multiple-Angle Incidence Resolution Spectrometry”

The Japan Society of Analytical Chemistry

19 August 2020

WAKAMIYA, Atsushi KANEMITSU, Yoshihiko

The 19th (2019) Green and Sustainable Chemistry Award “Awarded by the Minister of Education, Culture, Sports, Science and Technology”

“Development of Highly Efficient Perovskite Solar Cells”

Japan Association for Chemical Innovation

10 June 2020



NAKAMURA, Tomoya



ICR Award for Young Scientists

“Sn(IV)-free Tin Perovskite Films Realized by in situ Sn(0) Nanoparticle Treatment of the Precursor Solution”

Institute for Chemical Research, Kyoto University

11 December 2020

NAKAMURA, Masaharu



SSOCJ Nissan Chemical Corporation Award for New Reaction/Method in Organic Synthesis 2019

“Development of Iron-catalyzed Cross-coupling Reactions for the Synthesis of Functional Organic Compounds”

The Society of Synthetic Organic Chemistry, Japan

19 February 2020

SANARI, Yasuyuki



ICR Award for Graduate Students

“Modifying Angular and Polarization Selection Rules of High-order Harmonics by Controlling Electron Trajectories in k-Space”

Institute for Chemical Research, Kyoto University

11 December 2020

ZHANG, Ruixuan



The Best Oral Presentation Award

JSME Environmental Virus Meeting 2020

“Medusavirus Transcriptome & the Genome Characterization of a New Medusavirus Strain”

Japanese Society of Microbial Ecology

4 September 2020

Paper Awards

NISHIMURA, Tomoe



MSJ Paper Award

“Fabrication of Ferrimagnetic Co/Gd/Pt Multilayers with Structural Inversion Symmetry Breaking”

The Magnetics Society of Japan

16 January 2020

AKUTSU, Tatsuya *et al.*



Best Theory Paper Award

“A New Integer Linear Programming Formulation to the Inverse QSAR/QSPR for Acyclic Chemical Compounds Using Skeleton Trees”

Zhang, F.; Zhu, J.; Chiewvanichakorn, R.; Shurbevesk, A.; Nagamochi, H.; Akutsu, T.

The 33rd International Conference on Industrial, Engineering & Other Applications of Applied Intelligent Systems

25 September 2020

LI, Tian



MSJ Paper Award

“Chromatic Aberration Effect in Refraction of Spin Waves”

The Magnetics Society of Japan

19 November 2020

Poster Awards

IMAMURA, Yuji



Excellent Presentation Award

2020 KIPS Young Researchers Polymer Symposium

“Dual Control of Stereoregularity and Molecular Weight by the Hybridization of Reversible Deactivation Radical Polymerization with a Lanthanide Lewis Acid Catalyst”

Foundation of Institute for Chemical Fibers, Japan

23 October 2020

SATO, Takeshi



The Best Poster Award

“Multi-scale Simulation for Temperature Dependent Flows of Entangled Polymer Melts”

The 15th International Workshop for East Asian Young Rheologists (IWEAYR-15)

10 January 2020

TSUDZUKI, Taiku



Best Poster Award

The 21st Annual Meeting of Japanese Society for Extremophiles

“Regulation of Surface Structure of Extracellular Membrane Vesicles and Their Cargo Transport by Surface Polysaccharide Biosynthesis Enzyme of *Shewanella vesiculosa* HM13”

The Japanese Society for Extremophiles

1 November 2020

KANEKO, Hiroto



Poster Award

12th Workshop for Young Bioinformatician

“Marine Biodiversity from Space–Remote Sensing and Metagenomes”

Young Researchers Society for Bioinformatics

28 August 2020

Obituary

Professor Emeritus

Dr. KAJI, Keisuke (1939–2020)



Dr. Keisuke Kaji, Professor Emeritus of Kyoto University, passed away on April 6, 2020, at the age of 81.

Dr. Kaji was born in Kobe on 14th of February, 1939. After graduation from the Department of Industrial Chemistry, Faculty of Engineering, Kobe University in 1963, he continued his studies on polymer chemistry at the Graduate School of Engineering, Kyoto University for five years. Under the supervision of Professor Emeritus Ichiro Sakurada, he was granted a doctoral degree from Kyoto University in 1970 for his studies on the determination of elastic moduli of polymer crystals by an X-ray diffraction method. In 1968, he was appointed an instructor of Department of Polymer Chemistry, Faculty of Engineering, Kyoto University. On leave from the University, in the years 1976 to 1977, he stayed in the Institut für Physikalische Chemie, Johannes-Gutenberg-Universität Mainz (the University of Mainz, West Germany) as Wissenschaftlicher Mitarbeiter to work on neutron scattering of polymers in collaboration with Professor Dr. Erhard W. Fischer. Dr. Kaji was promoted to an Associate Professor in 1981, and to a full Professor of Kyoto University in 1988 and directed the Division of Polymer Materials Science, Laboratory of Fundamental Material Properties, Institute for Chemical Research.

During the past 40 years, Dr. Kaji's research interest encompassed a wide area in polymer science including fiber science. He is known as a pioneer of neutron scattering researches of polymers in Japan, and he applied this method as well as X-ray and light scattering methods for elucidating structure, dynamics and phase behavior of polymer materials to relate their microscopic and macroscopic behaviors. His scientific life started mainly with determining crystalline elastic moduli of various polymers by an X-ray scattering technique, which give the limiting values for super-high modulus fibers. In this connection he solved several problems of abnormal scattering from small polymer crystallites in the amorphous matrix as well. After Mainz, he applied inelastic neutron scattering techniques

to elucidate the origins of the glass transition and excess heat capacities in amorphous polymers. He is the first to perform systematic experiments on the structure of polyelectrolyte solutions, establishing the phase diagram as functions of the degree of polymerization and the concentration in their wide ranges and revealing the cause for the well-known anomalous behavior in reduced viscosity at very dilute concentrations. He also investigated the structure and its formation processes of poly(vinyl alcohol) gels, showing that the structure is controlled by a competition between the rates of the gelation and the phase separation. His researches on polymer crystallization are prominent. He discovered for the first time a completely new type of primary crystal nucleation, called spinodal decomposition (SD)-assisted crystal nucleation, which is greatly different from the usual homogeneous crystal nucleation. This distinct research has inspired many international investigations in this field. To promote this finding, he organized a project team on polymer crystallization as a coordinator of NEDO International Joint Research Project supported by New Energy and Industrial Technology Development Organization.

For his prominent studies on static and dynamic structure of polymers by neutron and X-ray scattering, he was awarded the Prize of the Society of Polymer Science, Japan in 1985. Dr. Kaji devoted himself to the Society of Fiber Science and Technology, Japan. He served as the Head of Kansai Branch in 1994, as the Chairperson of the Advanced Fiber Materials Research Committee in the years 1994 to 1995, and as the vice-President of the Society in the years 1999 to 2002. He has also devoted to the Society of Polymer Science, Japan as the Regional Manager of Kansai Branch since 1984 and as the Associate Editor of Polymer Journal since 1999.

His contribution to the University through both academic and administrative activities is gratefully acknowledged.

Obituary

Professor Emeritus

Dr. TAKEKOSHI, Hidekuni (1926–2020)

Dr. TAKEKOSHI, Hidekuni, Professor Emeritus of Kyoto University, passed away on January 11, 2020, at the age of 93.

Obituary

Professor Emeritus

Dr. MATSUI, Masakazu (1935–2020)

Dr. MATSUI, Masakazu, Professor Emeritus of Kyoto University, passed away on March 11, 2020, at the age of 84.



PUBLICATIONS

INTERNATIONAL
RESEARCH
COLLABORATIONS

SELECTED GRANTS

THESSES



PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

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Kunzmann, R.; Omatsu, Y.; Schnakenburg, G.; Espinosa Ferao, A.; Yanagisawa, T.; Tokitoh, N.; Streubel, R., A Synthetic Equivalent for Unknown 1,3-Zwitterions?-A K/OR Phosphinidenoid Complex with an Additional Si-Cl Function, *Chem. Commun.*, **56**, 3899-3902 (2020).

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DIVISION OF MATERIALS CHEMISTRY

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— Inorganic Photonics Materials —

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DIVISION OF BIOCHEMISTRY

— Biofunctional Design-Chemistry —

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Kanemitsu, Y.; Yamada, T.; Handa, T.; Nagai, M., Optical Responses of Lead Halide Perovskite Semiconductors, *Semicond. Sci. Technol.*, **35**, 093001 (2020).

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BIOINFORMATICS CENTER

— Chemical Life Science —

Endo, H.; Blanc-Mathieu, R.; Li, Y.; Salazar, G.; Henry, N.; Labadie, K.; de Vargas, C.; Sullivan, M. B.; Bowler, C.; Wincker, P.; Karp-Boss, L.; Sunagawa, S.; Ogata, H., Biogeography of Marine Giant Viruses Reveals Their Interplay with Eukaryotes and Ecological Functions, *Nat. Ecol. Evol.*, doi: 10.1038/s41559-020-01288-w (2020).

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Sakurai, T.; Nishiyama, H.; Nagai, T.; Goto, S.; Ogata, H.; Kudo, M., Deficiency of Gankyrin in the Small Intestine is Associated with Augmented Colitis Accompanied by Altered Bacterial Composition of Intestinal Microbiota, *BMC Gastroenterol.*, **20**(1), 12 (2020).

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Nishiyama, H.; Endo, H.; Blanc-Mathieu, R.; Ogata, H., Ecological Structuring of Temperate Bacteriophages in the Inflammatory Bowel Disease-affected Gut, *Microorganisms*, **8**, 1663 (2020).

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— **Mathematical Bioinformatics** —

Chen, Z.; Zhao, P.; Li, F.; Marquez-Lago, T. T.; Leier, A.; Revote, J.; Zhu, Y.; Powell, D. R.; Akutsu, T.; Webb, G. I.; Chou, K.-C.; Smith, A. I.; Daly, R. J.; Li, J.; Song, J., *iLearn: An Integrated Platform and Meta-learner for Feature Engineering, Machine-learning Analysis and Modeling of DNA, RNA and Protein Sequence Data*, *Brief. Bioinform.*, **21**, 1047-1057 (2020).

Mei, S.; Li, F.; Leier, A.; Marquez-Lago, T. T.; Giam, K.; Croft, N. P.; Akutsu, T.; Smith, A. I.; Li, J.; Rossjohn, J.; Purcell, A. W.; Song, J., *A Comprehensive Review and Performance Evaluation of Bioinformatics Tools for HLA Class I Peptide-binding Prediction*, *Brief. Bioinform.*, **21**, 1119-1135 (2020).

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Zhang, Y.; Yu, S.; Xie, R.; Li, J.; Leier, A.; Marquez-Lago, T. T.; Akutsu, T.; Smith, A. I.; Ge, Z.; Wang, J.; Lithgow, T.; Song, J.; Hancock, J., *PeNGaRoo, A Combined Gradient Boosting and Ensemble Learning Framework for Predicting Non-classical Secreted Proteins*, *Bioinformatics*, **36**, 704-712 (2020).

Chiewvanichakorn, R.; Wang, C.; Zhang, Z.; Shurbevski, A.; Nagamochi, H.; Akutsu, T., *A Method for the Inverse QSAR/QSPR Based on Artificial Neural Networks and Mixed Integer Linear Programming*, *ACM International Conference Proceeding Series*, 40-46 (2020).

Azam, N. A.; Chiewvanichakorn, R.; Zhang, F.; Shurbevski, A.; Nagamochi, H.; Akutsu, T., *A Novel Method for the Inverse QSAR/QSPR Based on Artificial Neural Networks and Mixed Integer Linear Programming with Guaranteed Admissibility*, *BIOINFORMATICS 2020 - 11th International Conference on Bioinformatics Models, Methods and Algorithms, Proceedings; Part of 13th International Joint Conference on Biomedical Engineering Systems and Technologies, BIOSTEC 2020*, 101-108 (2020).

Zhu, J.; Wang, C.; Shurbevski, A.; Nagamochi, H.; Akutsu, T., *A Novel Method for Inference of Chemical Compounds of Cycle Index Two with Desired Properties Based on Artificial Neural Networks and Integer Programming*, *Algorithms*, **13**, 124 (2020).

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Zeng, J.; Cai, H.; Akutsu, T., *Breast Cancer Subtype by Imbalanced Omics Data through A Deep Learning Fusion Model*, *ACM International Conference Proceeding Series*, 78-83 (2020).

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Liu, P.; Melkman, A. A.; Akutsu, T., *Extracting Boolean and Probabilistic Rules from Trained Neural Networks*, *Neural Netw.*, **126**, 300-311 (2020).

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— **Bio-knowledge Engineering** —

Dai, S.; You, R.; Lu, Z.; Huang, X.; Mamitsuka, H.; Zhu, S., *FullMeSH: Improving Large-scale MeSH Indexing with Full Text*, *Bioinformatics*, **36**, 1533-1541 (2020).

Wimalawarne, K.; Yamada, M.; Mamitsuka, H., *Scaled Coupled Norms and Coupled Higher-order Tensor Completion*, *Neural Comput.*, **32**, 447-484 (2020).

Liu, L.; Huang, X.; Mamitsuka, H.; Zhu, S., *HPOLabeler: Improving Prediction of Human Protein-phenotype Associations by Learning to Rank*, *Bioinformatics*, **36**, 4180-4188 (2020).

Nguyen, C. H., *Structured Learning in Biological Domain*, *J. Syst. Sci. Syst. Eng.*, **29**, 440-453 (2020).

Nakamura, A.; Takigawa, I.; Mamitsuka, H., *Efficiently Enumerating Substrings with Statistically Significant Frequencies of Locally Optimal Occurrences in Gigantic String*, *Proc. Conf. AAAI Artif. Intell.*, **34(4)**, 5240-5247 (2020).

You, R.; Liu, Y.; Mamitsuka, H.; Zhu, S., *BERTMeSH: Deep Contextual Representation Learning for Large-scale High-performance MeSH Indexing with Full Text*, *Bioinformatics*, **36(14)**, 4180-4188 (2020).

Strahl, J.; Peltonen, J.; Mamitsuka, H.; Kaski, S., *Scalable Probabilistic Matrix Factorization with Graph-based Priors*, *Proc. Conf. AAAI Artif. Intell.*, **34(4)**, 5851-5858 (2020).

HAKUBI PROJECT

—Synthesis and Exploration of Novel Charge Transition Oxide Materials for Future Multifunctional Devices—

Denis Romero, F.; Amano Patino, M. E.; Haruta, M.; Kurata, H.; Attfield, J. P.; Shimakawa, Y., Conversion of a Defect Pyrochlore into a Double Perovskite via High-pressure, High-temperature Reduction of Te^{6+} , *Inorg. Chem.*, **59**, 343-349 (2020).

INTERNATIONAL RESEARCH COLLABORATIONS

[Australia]

Charles Sturt University, School of Computing and Mathematics

Monash University, Biomedicine Discovery Institute

RMIT University, School of Engineering

The University of Queensland, School of Chemical Engineering

University of Sydney, Sydney Medical School

[China, P.R.]

China Pharmaceutical University, Institute of Pharmaceutical Science

Chinese Academy of Sciences, CAS-MPG Partner Institute for Computational Biology, Shanghai Institute of Nutrition and Health

Chinese Academy of Sciences, Changchun Institute of Applied Chemistry (CIAC)

Chinese Academy of Sciences, Institute of Plant Physiology and Ecology

Chinese Academy of Sciences, Northeast Institute of Geography and Agroecology

Fudan University, Department of Chemistry

Fudan University, Key Laboratory of Computational Neuroscience and Brain-Inspired Intelligence

Fudan University, School of Computer Science and Shanghai Key Lab of Intelligent Information Processing

Fudan University, School of Pharmacy

Fudan University, Shanghai Institute of Artificial Intelligence Algorithms and Institute of Science and Technology for Brain-Inspired Intelligence

Henan University, Institute of Plant Stress Biology

Peking University, Department of Chemical Biology

The University of Hong Kong, Department of Mathematics

[Finland]

Aalto University, Department of Computer Science

Tampere University, Faculty of Information Technology and Communication Sciences

[France]

Centre National de la Recherche Scientifique

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

Sorbonne Université, Institut Parisien de Chimie Moléculaire

Sorbonne University, École Normale Supérieure, PSL University, CNRS, Laboratory of Biomolecules

Université de Strasbourg, Institut de Physique et Chimie des Matériaux de Strasbourg

[Germany]

European Molecular Biology Laboratory

Freie Universität Berlin, Fachbereich Physik

Institut für Ressourcenökologi, Helmholtz-Zentrum Dresden-Rossendorf

Karlsruhe Institute of Technology, Institut für Organische Chemie

Karlsruhe Institute of Technology, Institute of Biological Interfaces

Technische Universität Dresden, Theoretical Chemistry

Université de Strasbourg, Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS)

University of Bonn, Institute for Inorganic Chemistry

[India]

Indian Institute of Technology Bombay, Department of Chemistry

[Israel]

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

[Italy]

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

[Korea, R.]

Yonsei University, Department of Chemistry, Spectroscopy Laboratory for Functional, π -Electronic Systems

[Norway]

University of Bergen, Department of Biology

[Spain]

Universidad Complutense, Departamento de Química Inorgánica, Facultad de C.C. Químicas

[Sweden]

Stockholm University, Department of Biochemistry and Biophysics

[Taiwan]

Academia Sinica, Institute of Earth Sciences

Academia Sinica, Research Center for Environmental Changes

National Chiao Tung University, Institute of Bioinformatics and Systems Biology

National Taiwan University, Center for Condensed Matter Sciences

National Taiwan University, Department of Chemistry and Advanced Research Center of Green Materials Science and Technology

[Thailand]

Chiang Mai University, Center of Excellent for Innovation in Chemistry (PERCH-CIC), Faculty of Science

Chiang Mai University, Department of Chemistry, Faculty of Science

Chiang Mai University, Department of Industrial Chemistry, Faculty of Science

Chiang Mai University, Material Science Research Center, Faculty of Science

[U.K.]

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

The University of St Andrews, School of Chemistry Organic Semiconductor Centre EaSTCHEM

[U.S.A.]

Baylor College of Medicine, Department of Biochemistry & Molecular Biology

National Institutes of Health (NIH), National Center for Biotechnology Information (NCBI), National Library of Medicine (NLM)

Stony Brook University, Department of Materials Science and Chemical Engineering

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

UCLA, Department of Physics and Astronomy

[Vietnam]

Duy Tan University, Institute of Research and Development

Vietnam Academy of Agricultural Sciences, Agricultural Genetics Institute

*The list shows the institutions with which papers are co-authored.

SELECTED GRANTS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Mizuhata, Y.
Creation of Novel Conjugated Molecules with Heavy Phenyl Anions as Building Blocks
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 March 2021

Tokitoh, N.; Mizuhata, Y.; Yukimoto, M.
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

Tokitoh, N.
Synthesis of Hexasilabenzene
Grant-in-Aid for Challenging Research (Pioneering)
28 June 2019–31 March 2022

Yukimoto, M.
Creation of Tautomerizable Heavy Group14-16 Double Bonded Compounds
Grant-in-Aid for Early-Career Scientists
1 April 2018–31 March 2022

— Structural Organic Chemistry —

Murata, Y.
Creation and Development of Nanoscale Laboratory
Grant-in-Aid for Scientific Research (S)
1 June 2017–31 March 2022

Hirose, T.
Synthesis of π -Extended Helical Aromatic Molecules Towards Creation of Novel Molecular Functions with Chirality
Grant-in-Aid for Scientific Research (C)
1 April 2018–31 March 2021

Hirose, T.
Creation of Multi-dimensional Chiral Assemblies Based on π -Expanded Helical Aromatic Ligands
Grant-in-Aid for Scientific Research on Innovative Area “Coordination Asymmetry”
1 April 2019–31 March 2021

Hashikawa, Y.
Creation of Carbon Nanocages toward Single Molecule Chemistry
Grant-in-Aid for Early-Career Scientists
1 April 2020–31 March 2022

Hashikawa, Y.
Construction of Higher Order Structures Integrated by Precisely Arranged Hydroxy Groups in a 3D Manner
Grant-in-Aid for Scientific Research on Innovative Area “Aquatic Functional Materials”
1 April 2020–31 March 2022

— Synthetic Organic Chemistry —

Kawabata, T.
Asymmetric Synthesis of Chiral Supramolecules towards Pioneering Novel Chemical Space
Research Grant from the Uehara Memorial Foundation
1 April 2020–31 March 2021

Ueda, Y.
Catalytic Asymmetric Synthesis of Inherently Chiral Calixarenes and Its Application to Unique Molecular Recognition
Grant-in-Aid for Scientific Research (C)
1 April 2020–31 March 2023

Morisaki, K.
Site-selective C-H Bond Functionalization
Grant-in-Aid for Early-Career Scientists
1 April 2019–31 March 2022

— Advanced Inorganic Synthesis —

Teranishi, T.
Nanoscale Element Replacement Science: Structural Transformation of Nanocrystalline Phases and Development of Novel Functions
Grant-in-Aid for Scientific Research (S)
26 June 2019–31 March 2024

Teranishi, T.
Novel Development of Asymmetry Chemistry in Inorganic Nanocrystals
Grant-in-Aid for Scientific Research on Innovative Area “Coordination Asymmetry”
1 July 2016–31 March 2021

Teranishi, T.
Synthesis of Magnetic Nanoparticles and Proposal of Guideline for High Performance Ferrite Magnets Aiming at Creation of Novel Magnet Materials
Element Strategy Initiative, MEXT
1 April 2012–31 March 2022

Abbreviations and acronyms

JST : Japan Science and Technology Agency
MEXT : Ministry of Education, Culture, Sports, Science and Technology
METI : Ministry of Economy, Trade and Industry
NEDO : New Energy and Industrial Technology Development Organization

Teranishi, T.
Development of Manufacturing Process Technology for Solar Hydrogen, etc. (Innovative Photocatalysts)
Artificial Photosynthesis Project, NEDO
1 April 2012–31 March 2022

DIVISION OF MATERIALS CHEMISTRY

— Polymer Controlled Synthesis —

Yamago, S.
New Organic Chemistry and Material Science of Curved π -Conjugated Molecules
Grant-in-Aid for Scientific Research (S)
1 April 2016–31 May 2020

— Nanospintronics —

Ono, T.
Development and Understanding Spintronic Phenomena in Ferromagnets
Grant-in-Aid for Scientific Research (S)
31 August 2020–31 March 2025

DIVISION OF BIOCHEMISTRY

— Biofunctional Design-Chemistry —

Futaki, S.
Intracellular Fate of Extracellular Fine Particles and the Control System
CREST (Core Research for Evolutionary Science and Technology), JST
1 October 2018–31 March 2024

Futaki, S.
Development of New Methods for Cytosolic Delivery of Bioactive Proteins
Grant-in-Aid for Scientific Research (A)
1 April 2018–31 March 2020

Imanishi, M.
Control of RNA Modification for Antivirus Activities
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2021

— Chemistry of Molecular Biocatalysts —

Yamaguchi, S.
Molecular Mechanisms for the Timing of the Production of Stem Cells in Plants
Grant-in-Aid for Scientific Research on Innovative Area “Principles of Pluripotent Stem Cells Underlying Plant Vitality”
30 June 2017–31 March 2022

— Molecular Biology —

Aoyama, T.
Plant Epidermal Cell Differentiation Regulated by the Transcription Factor GL2
Grant-in-Aid for Scientific Research (B)
1 April 2016–31 March 2020

— Chemical Biology —

Uesugi, M.
Chemical Biological Exploration of New Functions of Endogenous Lipid-related Molecules
AMED-CREST
1 October 2014–31 March 2020

Uesugi, M.
Chemical Signals of Synthetic Nutrient Conjugates
Grant-in-Aid for Scientific Research on Innovative Areas
1 July 2017–31 March 2022

Uesugi, M.
Exploration of Self-assembling Bioactive Small Molecules
Grant-in-Aid for Scientific Research (A)
1 April 2019–31 March 2022

Uesugi, M.
Asian Chemical Biology Initiative
Core-to-Core Program, JSPS
1 April 2019–31 March 2022

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

Takemoto, Y.
Spatiotemporal Regulation of Protein Degradation by Small Molecule Compound and Light
Grant-in-Aid for Scientific Research (C)
1 April 2019–31 March 2022

DIVISION OF ENVIRONMENTAL CHEMISTRY

— Molecular Materials Chemistry —

Kaji, H.
Construction of Basic Science of Organic Devices by Precise Structural Analysis and Theoretical Chemical Calculation
Grant-in-Aid for Scientific Research (A)
1 April 2017–31 March 2020

Shizu, K.
Singlet Fission Materials by Engineering Inter-exciton Vibronic Coupling
Grant-in-Aid for Scientific Research (C)
1 April 2019–31 March 2021

Suzuki, K.
Structural Analysis of Organic Semiconducting Materials Using DNP-NMR
Grant-in-Aid for Early-Career Scientists
1 April 2019–31 March 2021

— Hydrospheric Environment Analytical Chemistry —

Sohrin, Y.
Ocean Section Study on the Basis of Stoichiometry and Stable Isotope Ratio of Trace Metals
Grant-in-Aid for Scientific Research (A)
1 April 2019–31 March 2023

Takano, S.
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

Takano, S.
Revealing Biogeochemical Cycles of Trace Metals Based on Isotopic Analysis of Sinking Particles
Mitsumasa Ito Memorial Research Grant, Research Institute for Ocean Chemistry Foundation
1 April 2020–31 March 2021

Zheng, L.
Sectional Distributions of Trace Metals in the South Pacific Ocean and the Indian Ocean
Mitsumasa Ito Memorial Research Grant, Research Institute for Ocean Chemistry Foundation
1 April 2020–31 March 2021

— **Chemistry for Functionalized Surfaces** —

Hasegawa, T.
Development of ROA Imaging and Its Application to Visualization of Atropisomers for a Study of Fluoroorganic Chemistry
Grant-in-Aid for Scientific Research (A) “Analytical Chemistry”
1 April 2015–31 March 2020

Shimoaka, T.
Molecular Interaction Analysis for Understanding Perfluoroalkyl Compound-Specific Properties
Grant-in-Aid for Young Scientists (B) “Analytical Chemistry”
1 April 2017–31 March 2020

Shioya, N.
Development of Multiple-Angle Incidence Resolution Reflection Spectrometry and Its Application to Organic Thin-Film Devices
Grant-in-Aid for Early-Career Scientists “Analytical Chemistry”
1 April 2019–31 March 2022

— **Molecular Microbial Science** —

Kurihara, T.
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, T.
Diversity of Acyl Groups of Phospholipids in Bacterial Cell Membranes: Its Generation Mechanism and Physiological Significance
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 March 2021

Kurihara, T.
Elucidation of the Mechanism of Selective Protein Transport to Bacterial Extracellular Membrane Vesicles and Their Application for Construction of an Extracellular Platform for Protein Production
A Large Research Grant from the Institute for Fermentation, Osaka
1 April 2019–31 March 2021

Kawamoto, J.
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

Ogawa, T.
Exploration and Functional Elucidation of a Novel Protein Involved in the Metabolism of ω -3 Polyunsaturated Fatty Acids in Bacteria
Grant-in-Aid for Early-Career Scientists
1 April 2019–31 March 2021

Ogawa, T.
Research on Bacterial Conversion of ω -3 Polyunsaturated Fatty Acids and its Application
A General Research Grant from the Institute for Fermentation, Osaka
1 April 2019–31 March 2021

DIVISION OF MULTIDISCIPLINARY CHEMISTRY
— **Molecular Rheology** —

Watanabe, H.
Unified Understanding of the Polymer Dynamics under Elongational and Shear Flows
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

— **Molecular Aggregation Analysis** —

Wakamiya, A.
Development of High Performance and Environmentally Friendly Perovskite Type Solar Cells
ALCA (Advanced Low Carbon Technology Research and Development Program), JST
16 November 2016–31 March 2021

Wakamiya, A.
Research and Development of Film Photovoltaics
Center of Innovation (COI) Program, JST
1 November 2013–31 March 2021

Wakamiya, A.
Research and Development of Film Type Perovskite Photovoltaics with Highly Flexible Design
Development of Multi-purpose Thin Film Perovskite Solar Module Technologies, NEDO
13 July 2020–31 March 2023

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE
— **Particle Beam Science** —

Wakasugi, M.
Development of an Unstable-nuclear Target for the Nuclear-reaction Study with Rarely Produced Nuclei
Grant-in-Aid for Challenging Exploratory Research (Pioneering)
1 April 2020–31 March 2023

Tsukada, K.
Isotope Dependences of Nuclear Charge Distributions and Neutron Radius by Electron Scattering
Grant-in-Aid for Scientific Research (A)
1 April 2020–31 March 2025

Ogawara, R.
Development of Prototype Device for Ion Extraction System with Resonant Oscillation
Grant-in-Aid for Early-Career Scientists
1 April 2020–31 March 2022

— **Electron Microscopy and Crystal Chemistry** —

Kurata, H.
Advanced Characterization Nanotechnology Platform at Kyoto University
Nanotechnology Platform Project, MEXT
2 July 2012–31 March 2022

Kurata, H.
Development of Precise Spatially Resolved EELS and Analysis of Interfacial Electronic States
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2020

Kurata, H.
Electronic Structure Analysis by Aloof Beam EELS
Grant-in-Aid for Challenging Research
1 April 2019–31 March 2022

Haruta, M.
High Spatical and Energy Resolution Electronic State Mapping
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— **Synthetic Organotransformation** —

Nakamura, M.
Application and Verification of Quantum Control in Iron-catalyzed Cross-coupling Reaction
Grant-in-Aid for Scientific Research (B)
1 April 2020–31 March 2023

Nakamura, M.
Development of Selective Woody Molecular Transformations for Forest Chemical Industry
Grant-in-Aid for Challenging Research (Exploratory)
29 June 2018–31 March 2020

Takaya, H.
Artificial Enzymes Base on Metalated Peptides
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2020

— **Advanced Solid State Chemistry** —

Shimakawa, Y.
High-pressure Synthesis of Novel Transition-metal Oxides and Exploring Their Functional Properties
Grant-in-Aid for Scientific Research (A)
1 April 2020–31 March 2024

— **Nanophotonics** —

Kanemitsu, Y.
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, Y.
Design of Next-generation Flexible Photonic Devices Based on Metal Halide Perovskites
CREST (Core Research for Evolutionary Science and Technology), JST
1 October 2016–31 March 2022

Hirori, H.
Development of Time-resolved THz-STM Working at Low Temperature and High Magnetic Field
The Mitsubishi Foundation
10 July 2019–31 May 2021

BIOINFORMATICS CENTER

— **Chemical Life Science** —

Ogata, H.
Deciphering the Mechanisms of Virus-host Co-existence in Aquatic Environments
Grant-in-Aid for Scientific Research on Innovative Area “Neovirology, the Raison d’Etre of Viruses”
30 June 2016–31 March 2021

Ogata, H.
The Biosphere of Aggregated Particles: Elucidating the Regulatory Mechanisms of Marine Carbon Cycles
Grant-in-Aid for Scientific Research (S)
3 July 2019–31 March 2023

Ogata, H.
Comprehensive Study and Establishment of Application Foundation of Carboxydrotrophic Bacteria through Spatio-temporal Search
Grant-in-Aid for Scientific Research (S)
1 April 2016–31 March 2021

Ogata, H.
Comprehensive Understanding of the Role of Giant Viruses in Aquatic Ecosystems
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 March 2022

Ogata, H.
Comprehensive Understanding of Ecology and Virus-host Interactions of Giant Viruses in Aquatic Ecosystems
Grant-in-Aid for Scientific Research (B)
1 April 2020–31 March 2023

Ogata, H.
Virus-host Database
Grant-in-Aid for Publication of Scientific Research Results (Database)
1 April 2020–31 March 2025

Endo, H.
Integrative Understanding of Marine Nitrogen Fixation Based on Global Observations from Tropics to Polar Regions
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

Endo, H.
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 2022

— **Mathematical Bioinformatics** —

Akutsu, T.
Analysis and Application of Discrete Preimage Problems
Grant-in-Aid for Scientific Research (A)
1 April 2018–31 March 2023

Tamura, T.
Efficient Algorithms for Design of Metabolic Networks for
Valuable Metabolite Production
Grant-in-Aid for Scientific Research (B)
1 April 2020–31 March 2025

Mori, T.
Development of Cell Trajectory Inference and Comparison Algo-
rithm Based on Single-cell Omics Data
Grant-in Aid for Early-Career Scientists
1 April 2019–31 March 2021

— **Bio-knowledge Engineering** —

Mamitsuka, H.
Efficient Estimation of Data Structure from Multiple Tensors
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

Nguyen, C. H.
Machine Learning on Large Graphs
Grant-in-Aid for Scientific Research (C)
1 April 2018–31 March 2021

THESES

- ANDO, Fuyuki
D Sc, Kyoto University
“Microscopic Understanding of Electric Effects in Co Magnetism”
Supervisor: Prof ONO, Teruo
17 January 2020
- ARAFILES, Jan Vincent V.
D Pharm Sc, Kyoto University
“Macropinocytosis-inducing Peptides: Identification, Utility, and Mechanism-of-Action”
Supervisor: Prof FUTAKI, Shiroh
23 September 2020
- CHEN, Chen
D Agr, Kyoto University
“Studies on Selective Protein Loading onto Extracellular Membrane Vesicles of a Novel Cold-adapted Bacterium, *Shewanella vesiculosa* HM13”
Supervisor: Prof KURIHARA, Tatsuo
23 March 2020
- FURUTA, Tomoyuki
D Med, Kyoto University
“Nutrient-based Chemical Library as a Source of Energy Metabolism Modulators”
Supervisor: Prof UESUGI, Motonari
23 September 2020
- GONDOH, Naruhiro
D Pharm Sc, Kyoto University
“Development of Site-selective C-C Bond and Enantioselective C-O Bond Formation Reaction by Organocatalysis”
Supervisor: Prof KAWABATA, Takeo
24 March 2020
- HANDA, Taketo
D Sc, Kyoto University
“Electron-phonon Interactions and Thermo-optic Properties of Metal Halide Perovskites”
Supervisor: Prof KANEMITSU, Yoshihiko
23 March 2020
- KAWAI, Soichiro
D Agr, Kyoto University
“Development of Low-temperature Protein Production Systems by Using Cold-adapted Bacteria, *Shewanella livingstonensis* Ac10 and *Pseudoalteromonas nigrifaciens* Sq02”
Supervisor: Prof KURIHARA, Tatsuo
23 September 2020
- KAWASAKI, Naohiko
D Sc, Kyoto University
“Analysis of Electronic Structure and Dielectric Properties of Materials in the Nanometer Region by Electron Energy Loss Spectroscopy and Theoretical Calculations”
Supervisor: Prof KURATA, Hiroki
23 March 2020
- KUBO, Shosei
D Eng, Kyoto University
“Theoretical and Experimental Studies of Organic Semiconductors”
Supervisor: Prof KAJI, Hironori
23 March 2020
- MASUDA, Toshihiro
D Pharm Sc, Kyoto University
“Control of Cellular Functions via Interaction between Amphiphilic Peptides and Cell Membrane”
Supervisor: Prof FUTAKI, Shiroh
23 March 2020
- NGUYEN, Dai Hai
D Pharm Sc, Kyoto University
“Machine Learning for Metabolite Identification with Mass Spectrometry Data”
Supervisor: Prof MAMITSUKA, Hiroshi
23 September 2020
- NISHIMURA, Tomoe
D Sc, Kyoto University
“Magnetization Dynamics Using Ferrimagnetic Thin Films”
Supervisor: Prof ONO, Teruo
17 January 2020
- ODA, Kento
D Sc, Kyoto University
“Detection of Neel Vectors in Antiferromagnets by Spin Transport Phenomena”
Supervisor: Prof ONO, Teruo
17 January 2020
- OKUNO, Takaya
D Sc, Kyoto University
“Magnetic Dynamics in Antiferromagnetically-coupled Ferrimagnets: The Role of Angular Momentum”
Supervisor: Prof ONO, Teruo
17 January 2020
- PARK, Beomsu
D Eng, Kyoto University
“Development of New Stereocontrolled Radical Polymerization Using Acid Catalysts”
Supervisor: Prof YAMAGO, Shigeru
24 November 2020
- PUNZALAN, Louvy Lynn Calvelo
D Med, Kyoto University
“Chemoproteomic Profiling of a Pharmacophore-focused Chemical Library”
Supervisor: Prof UESUGI, Motonari
23 September 2020
- SHIBAYAMA, Hiromitsu
D Pharm Sc, Kyoto University
“Unified Total Syntheses of Ellagitannins based on Sequential Site-selective Functionalization of Unprotected Glucose”
Supervisor: Prof KAWABATA, Takeo
24 March 2020

SUN, Liansheng
D Eng, Kyoto University
“Studies on the Syntheses and Properties of Cycloparaphenylenes
Having Heteroatom Functionalities and New Topology”
Supervisor: Prof YAMAGO, Shigeru
25 May 2020

TSUJISAKA, Makoto
D Sc, Kyoto University
“Development of Stable Isotope Ratio Analysis for Molybdenum
and Tungsten in Sediments and Its Application to Paleoceanographic
Study of the Japan Sea”
Supervisor: Prof SOHRIN, Yoshiki
23 March 2020

WADA, Yoshimasa
D Eng, Kyoto University
“Molecular Design and Realization of Highly Efficient Thermally
Activated Delayed Fluorescence Emitters for Organic Light-emitting
Diodes”
Supervisor: Prof KAJI, Hironori
23 March 2020

YANAGISAWA, Tatsuya
D Sc, Kyoto University
“Studies on Single-bond Compounds between Heavier Group
13/15 Elements toward Small Molecule Activation”
Supervisor: Prof TOKITOH, Norihiro
23 March 2020

YOKOYAMA, Fumiaki
D Agr, Kyoto University
“Studies on Production Mechanisms of Extracellular Membrane
Vesicles of Cold-adapted Bacteria”
Supervisor: Prof KURIHARA, Tatsuo
23 March 2020

YOSHIKAWA, Genki
D Sc, Kyoto University
“Comparative and Evolutionary Genome Analysis for Giant
Viruses”
Supervisor: Prof OGATA, Hiroyuki
23 March 2020



**THE 120TH
ICR ANNUAL
SYMPOSIUM**

SEMINARS

**MEETINGS AND
SYMPOSIA**



THE 120TH ICR ANNUAL SYMPOSIUM

(11 December 2020)

ORAL PRESENTATION

MASHIGUCHI, Kiyoshi (Chemistry of Molecular Biocatalysts)
“Analysis of Strigolactone Biosynthesis and Transport”

YUKIMOTO, Mariko (Organoelement Chemistry)
“Synthesis of Highly Reactive Germanium Compounds Utilizing a TbtCH₂ Group”

MORI, Tomoya (Mathematical Bioinformatics)
“*In Silico* 3D Tissue Reconstruction of Mid-gastrula Mouse Embryo by Self-organizing Map”

AMANO PATINO, Midori Estefani (Advanced Solid State Chemistry)
“Synthesis and Magnetic Property Characterization of the Quadruple Perovskite CaFe₃Ti₄O₁₂”

SATO, Takeshi (Molecular Rheology)
“Development of a Coarse-grained Simulation Model for Predicting Rheology”

— ICR Award for Young Scientists —

SHIOTA, Yoichi (Nanospintronics)
“Tunable Magnon-magnon Coupling Mediated by Dynamic Dipolar Interaction in Synthetic Antiferromagnets”

ZHENG, Linjie (Hydrospheric Environment Analytical Chemistry)
“Distinct Basin-scale-distributions of Aluminum, Manganese, Cobalt, and Lead in the North Pacific Ocean”

NAKAMURA, Tomoya (Molecular Aggregation Analysis)
“Sn(IV)-free Tin Perovskite Films Realized by *in situ* Sn(0) Nanoparticle Treatment of the Precursor Solution”

— ICR Award for Graduate Students —

ISHIBASHI, Mio (Nanospintronics)
“Switchable Giant Nonreciprocal Frequency Shift of Propagating Spin Waves in Synthetic Antiferromagnets”

SANARI, Yasuyuki (Nanophotonics)
“Modifying Angular and Polarization Selection Rules of High-order Harmonics by Controlling Electron Trajectories in *k*-Space”

— ICR Grants for Promoting Integrated Research —

KAWANO, Kenichi (Biofunctional Design-Chemistry)
“Development of a High-throughput Detection Method for Bacterial Extracellular Membrane Vesicles Using a Curvature-sensing Peptide”

POSTER PRESENTATIONS

LW: Laboratory Whole Presentation

LT: Laboratory Topic

GE: General Presentation

— Organoelement Chemistry —

LW “Studies on the Synthesis and Properties of Novel Organic Compounds Containing Heavier Elements”

— Structural Organic Chemistry —

LW “Research Activities in Structural Organic Chemistry Laboratory”

— Synthetic Organic Chemistry —

LW “Recent Research of Division of Synthetic Chemistry”

GE MORISAKI, Kazuhiro; EMI, Ryota; SATO, Yuki; CHEN, Gong; UJI, Akihito; UEDA, Yoshihiro; KAWABATA, Takeo
“Remote Asymmetric Induction by C(sp²)-H Amination”

— Advanced Inorganic Synthesis —

LT “Current Research Topics in Advanced Inorganic Synthesis”

GE NAKAGAWA, Fumiko; SARUYAMA, Masaki; TERANISHI, Toshiharu
“One-pot Synthesis of Assembly-controlled Nanoparticle Superstructures”

— Chemistry of Polymer Materials —

LW “Research Activities in Laboratory of Polymer Materials Chemistry”

GE SAITO, Masahiro; SAKAKIBARA, Keita; TSUJII, Yoshinobu
“Swelling Characteristics of Concentrated Polymer Brushes Studied by *in-situ* Measurement of Film Thickness on Spinning”

— Polymer Controlled Synthesis —

LW “Introduction of Research in the Field of Polymer Controlled Synthesis”

GE TERABAYASHI, Tomoaki; KAYAHARA, Eiichi; KATO, Tatsuhisa; YAMAGO, Shigeru
“Syntheses and Properties of Mobius and Double-twisted Cycloparaphenylene Derivatives”

GE IMAMURA, Yuji; YAMAGO, Shigeru
“Dual Control of Molecular Weight and Stereoregularity of Polyacrylamides by TERP in the Presence of Lanthanide Lewis Acids”

GE HE, Yuzhong; LU, Yangtian; YAMAGO, Sigeru
“Synthesis and Properties of Amphiphathic Block Copolymers Having Hyperbranched Structures”

GE JIANG, Yuhan; TOSAKA, Masatoshi; TSUJISAKA, Makoto; SOHRIN, Yoshiki; YAMAGO, Shigeru
“A Method for Removal of Organotellurium Group from the Polymers Prepared by *ab-initio* Emulsion Organotellurium-mediated Radical Polymerization”

GE LI, Xiaopei; OGIHARA, Tasuku; NAKAMURA, Yasuyuki; YAMAGO, Shigeru
“Evidence for Polarity- and Viscosity-controlled Domains in the Termination Reaction in the Radical Polymerization of Acrylonitrile”

— Inorganic Photonics Materials —

LW “Research Progress at Inorganic Photonic Lab”

— Nanospintronics —

LW “Recent Progress in Nanospintronics Lab”

GE IKEBUCHI, Tetsuya
“Crystal Orientation Dependence of Spin Hall Angle in Epitaxial Pt/Py Films”

GE HUNG, Yu Min
“Low Current Driven Vertical Domain Wall Motion Memory with Artificial Ferromagnet”

— Biofunctional Design-Chemistry —

LW “Research in the Biofunctional Design-Chemistry Laboratory”

GE SAKAMOTO, Kentarou; AKISHIBA, Misao; IWATA, Takahiro; MICHIBATA, Junya; IDE, Akiko; KAWANO, Kenichi; FUTAKI, Shiroh
“Creation of Endosomolytic Peptide ‘HAad’ and Its Analog with Improved Cytosolic Macromolecule Delivering Activity”

— Chemistry of Molecular Biocatalysts —

LW “Research Activities in Laboratory of Chemistry of Molecular Biocatalysts”

— Molecular Biology —

LW “Research Projects in the Laboratory of Molecular Biology”

— Chemical Biology —

LW “Create New World of Bioactive Synthetic Molecules”

— Molecular Materials Chemistry —

LW “Research Activities in Molecular Materials Chemistry Laboratory”

GE KUSAKABE, Yu
“Conformation Control of Iminodibenzyl-based Thermally Activated Delayed Fluorescence Material by tilted Face-to-Face Alignment with Optimal Distance (tFFO) Design”

GE MORIWAKI, Kazuki
“Multiscale Simulation of Charge Transport in Host-guest-based Emission Layer of Organic Light-emitting Diodes”

— Hydrospheric Environment Analytical Chemistry —

LW “Reveal the Ocean by Using Trace Elements and Their Isotopes”

GE NAGAE, Ayumi; TAKANO, Shotaro; SOHRIN, Yoshiki
“Sectional Distribution of Stable Isotope Ratios for Dissolved Nickel, Copper, and Zinc in the Subarctic North Pacific”

— Chemistry for Functionalized Surfaces —

LW “Study on Two-dimensional Molecular Aggregate Bridging the Molecular Structure and Material Properties”

GE YOSHIDA, Mariko; SHIOYA, Nobutaka; FUJII, Masamichi; SHIMOAKA, Takafumi; HASEGAWA, Takeshi
“Disappearance of Odd-Even Effect of n-Alkanes in a Thin Film”

GE OOTSUKI, Masashi; SHIMOAKA, Takafumi; SHIOYA, Nobutaka; HASEGAWA, Takeshi
“Raman Spectroscopic Analysis of the Surface on a Microcrystal of Perfluoroalkane”

— Molecular Microbial Science —

LW “Microbial Science Laboratory”

GE SUWANAWAT, Nittikarn; KUBOSHIMA, Misaki; KAWAMOTO, Jun; OGAWA, Takuya; KURIHARA, Tatsuo
“Studies on the Lysophosphatidic Acid Acyltransferase Homologs of *Shewanella livingstonensis* Ac10”

— Polymer Materials Science —

LW “An Introduction to Takenaka Lab”

GE MITANI, Kenta; OGAWA, Hiroki; WATANABE, Yuki; NISHIKAWA, Yukihito; MASHITA, Ryo; TAKENAKA, Mikihito
“Visualization of the Distribution of Oriented Nanoparticle Fillers and Voids in Rubber/Filler Under Strain”

GE KUMAGAWA, Daiki; TAKENAKA, Mikihito; WATANABE, Yuki; INOUE, Tadashi
“Structure-property Relationship in Rubber/Filler Systems”

GE ODA, Tappei; TAKENAKA, Mikihito; TERASHIMA, Takaya; HIRAI, Tomoyasu
“Ordered Structures of an Asymmetric Diblock Copolymer”

— **Molecular Aggregation Analysis** —

[LW] “Research Progress in Molecular Aggregation Analysis Laboratory”

— **Particle Beam Science** —

[LW] “Research at Particle-Beam Science Laboratory”

— **Laser Matter Interaction Science** —

[LW] “Research Activities in Laboratory of Laser Matter Science”

[GE] FURUKAWA, Yuki; INOUE, Shunsuke; HASHIDA, Masaki
“Development of a Method to Measure the Depth-directional Distribution of Absorption Coefficient of Metal Surface Irradiated by Ultrashort Laser Pulse”

— **Electron Microscopy and Crystal Chemistry** —

[LW] “Research Activities in Division of Electron Microscopy and Crystal Chemistry”

[GE] IWASHIMIZU, Chisaki; HARUTA, Mitsutaka; KURATA, Hiroki
“Electron Orbital Mapping Using STEM-EELS”

— **Atomic and Molecular Structures** —

[LW] “Introduction of Atomic and Molecular Structures Laboratory”

— **Synthetic Organotransformation** —

[LW] “Introduction of Synthetic Organotransformation Group”

[GE] SHARMA, Akhilesh K.; ISEGAWA, Miho; SUZUKI, Tsuyoshi; HATAKEYAMA, Takuji; MOROKUMA, Keiji; NAKAMURA, Masaharu
“Delineating Mechanism of Iron-catalyzed Amination Reaction Using DFT Method”

— **Advanced Solid State Chemistry** —

[LW] “Research Introduction in Advanced Solid State Chemistry Laboratory”

— **Organometallic Chemistry** —

[LW] “Activity Report: Organometallic Chemistry Laboratory”

[GE] WAKIOKA, Masayuki; YAMASHITA, Natsumi; OZAWA, Fumiyouki
“Stereo-controlled Synthesis and *cis-trans* Isomerization of *cis*-Polythienylenevinylene”

— **Nanophotonics** —

[LW] “Recent Research Topics of Nanophotonics Group”

— **Chemical Life Science** —

[LW] “Introduction of Chemical Life Science”

— **Mathematical Bioinformatics** —

[LT] WANG, Feiqi
“Comparison of Pseudoknotted RNA Secondary Structures by Topological Centroid Identification and Tree Edit Distance”

— **Bio-knowledge Engineering** —

[LT] NGUYEN, Canh Hao; MAMITSUKA, Hiroshi
“Sparse Learning on Hypergraphs”

SEMINARS

Assoc Prof CONVERTINO, Matteo
Faculty of Information Science and Technology, Gi-CoRE Station
for Big Data & Cybersecurity, Hokkaido University, Hokkaido,
Japan
“Ecosystem Nexus: from *E.coli* to Ocean Bacterioplankton
Collective Patterns”
16 July 2020

Prof ISHIDA, Yasuhiro
RIKEN, Saitama, Japan
“More Haste, Less Speed: Precision Synthesis of Soft Materials”
30 January 2020

Assoc Prof KOSONO, Saori
Biotechnology Research Center, The University of Tokyo, Tokyo,
Japan
“Challenges and Prospects of Bacterial Protein Acylation Re-
search”
21 February 2020

Dr NARITA, Hideki
Graduate School of Science, Kyoto University, Kyoto, Japan
“Novel Phenomena in Chiral Magnets”
17 September 2020

Assoc Prof SUNADA, Yusuke
Institute of Industrial Science, The University of Tokyo, Tokyo,
Japan
“Iron Catalysts and Metallic Clusters through Cooperation of
Metal and Silicon Atoms”
27 October 2020

Prof SUNG, Wing-Kin
Department of Computer Science, School of Computing, National
University of Singapore/Genome Institute of Singapore, Singapore
“Finding Deletion, Tandem Duplication and Virus Integration
Using High-throughput Sequencing Data”
22 January 2020

Prof TOMITA, Etsuji
The Advanced Algorithms Research Laboratory, The University
of Electro-Communications, Tokyo, Japan
“The Maximum Clique Problem and Its Applications”
7 February 2020

Mr UEDA, Kento
The University of Tokyo, Tokyo, Japan
“Quantum Transport in Superconductor-Semiconductor Josephson
Junctions”
1 April 2020

Prof VERT, Jean-Philippe
Google Brain in Paris/Centre for Computational Biology at Mines
ParisTech, France
“Computational Analysis of Tumour Heterogeneity, from Bulk to
Single-cell Genomics”
22 January 2020

Prof YAMADA, Hiroko
Nara Institute of Science and Technology, Nara, Japan
“Synthesis of Functional Materials Using the Precursor Approach”
7 October 2020

MEETINGS AND SYMPOSIA

The 15th International Workshop for East Asian Young Rheologists (IWEAYR-15)

Co-organized by WATANABE, Hiroshi
8–10 January 2020 (Changchun, China, P.R.)

2020 10th International Conference on Bioscience, Biochemistry and Bioinformatics (ICBBB 2020)

Organized by AKUTSU, Tatsuya
19–22 January 2020 (Kyoto, Japan)

Workshop in IIBMP2020, Analysis and Control of Metabolic Networks

Organized by TAMURA, Takeyuki
2 September 2020 (Online)

Environmental Virus Meeting 2020

Organized by ENDO, Hisashi
4 September 2020 (Kyoto, Japan)

74th Annual Autumn Meeting of the Research Institute for Oceanochemistry Foundation

Organized by SOHRIN, Yoshiki
14 November 2020 (Kyoto, Japan)

Shanghai-Kyoto Chemistry Forum 2020

Organized by UESUGI, Motonari
20 December 2020 (Online)



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