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Kyoto University



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

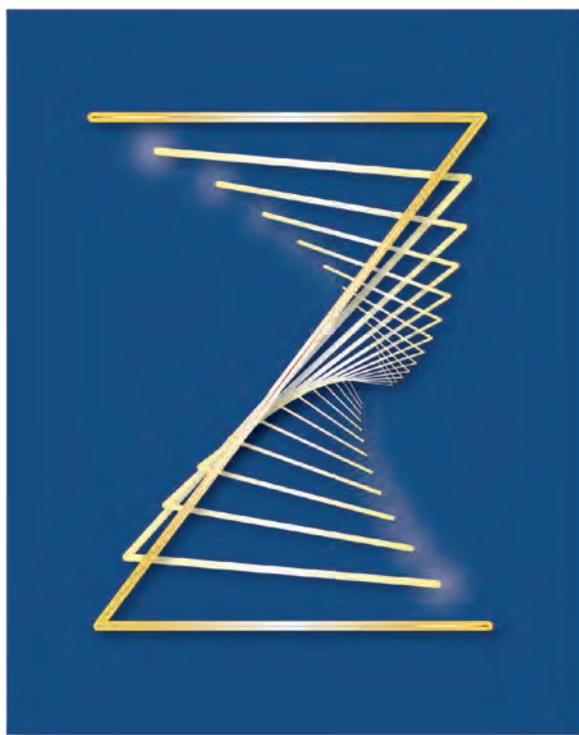
ICR has established a fund called "The ICR's 100th Anniversary Fund," which is a part of the Kyoto University Fund. Its aims are to hold the 100th anniversary event in 2026, to enhance the educational and research environments at ICR, and to promote social contribution activities.

We ask for your kind understanding and cooperation.



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

**ICR
ANNUAL
REPORT
2021**



**Institute for Chemical Research
Kyoto University**
Volume 28



Preface

The Institute for Chemical Research (ICR) was founded in 1926 as the first research institute of Kyoto University. Its founding vision was “To Excel in the Investigation of 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, 190 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) *Tracing the Incorporation of the “9th Sulfur” into the Nitrogenase Cofactor Precursor*; 2) *Determinants of Crystal Structure Transformation of Ionic Nanocrystals in Cation Exchange Reactions*; 3) *Iron-catalysed Enantioselective Carbometalation of Azabicycloalkenes*; 4) *Mixed Lead–Tin Perovskite Films with $>7 \mu\text{s}$ Charge Carrier Lifetimes*; 5) *Facile Cytosolic Translocation of IgG in the Presence of Attenuated Cationic Amphiphilic Lytic Peptides*; 6) *Giant Multiple Caloric Effects in Charge Transition Ferrimagnet*; 7) *Diamond Sensors with Ultra-high Dynamic Range Quantum Measurements Retaining Its Sensitivity*. Some other topics were also presented in the 121st ICR Annual Symposium on December 10, 2021.

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, and *Uji-Campus Base of Equipment Support* for reinforcing research infrastructure. We also promote international collaboration with overseas universities/institutions (with 69 official international collaboration agreements). In chemistry-oriented fields, ICR has maintained the global activities as a MEXT-certified *International Joint Usage/Research Center* since 2018 and a Kyoto University-approved *On-site Laboratory*, the “*Kyoto University Shanghai Lab*” in Shanghai, China since 2019. 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. Additionally in this year, ICR has established and contributed to a *Center for Spintronics Research Network (CSRN)* and the *Biomass Product Tree Industry-Academia Collaborative Research Laboratory* to strengthen research activities in collaboration with other institutions.

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 “Innovation” and “Integrity” 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 2022

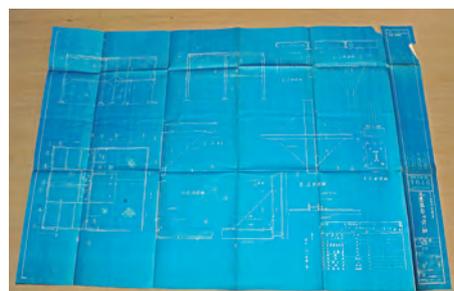
TSUJII, Yoshinobu
Director

ICR News 2021

Important Historical Material on Chemical Technology Recognized by the National Museum of Nature and Science

■ Prof MURATA, Yasujiro

The National Museum of Nature and Science, under the auspices of the Research Committee on the History of Industrial Technology, conducted a five-year research project from 1997 on the evaluation, preservation, and disclosure of materials on the history of industrial technology, with the cooperation of industry, academia, and government. In addition to creating a database of where and how materials showing the development of Japan's industrial technology remain, the research has examined the systematization of technology, the registration of materials, the networking of information on the history of industrial technology, and the formation of a new academic field on technological innovation. Based on these results, the History of Industrial Technology Research Committee formulated a concept in August 2001 that an information center for "the history of industrial technology to be useful for the future" needs to be established. Based on this concept, the National Museum of Nature and Science established the "Information Center for the History of Industrial Technology" in June 2002, and opened the center in June 2003. On September 14, 2021, the Fischer-Tropsch synthetic catalyst, prototypes, and related materials stored at the Institute of Chemical Research were recognized as the 302nd important historical material on chemical technology.



Collaboration between Quantum Beam Analysis Alliance and Kyoto University Begins

■ Prof TAKENAKA, Mikihiro

On August 23, the "Quantum Beam Analysis Alliance" (Representative: Mikihiro Takenaka; Institute for Chemical Research, Kyoto University) signed an agreement with the Office of Society Academia Collaboration for Innovation of Kyoto University for the use of the Kyoto University Beamline at the SPring-8. This agreement will enable us to achieve strong collaboration between industry, academia, and facilities, and to develop human resources for quantum beam research in the industry using the Kyoto University Beamline at SPring-8.

As part of the FY2021 feasibility period, "Quantum Beam Analysis Alliance" has completed a joint experiment on XAFS and SAXS at Kyoto University Beamline and has conducted activities to acquire the skills of members of participating companies. The alliance has also started to deliver online classes by leading experts in various quantum beam techniques.

In 2022, the alliance aims to establish and operate a course called "Quantum Beam Research Division". With this new course as a starting point, the alliance will further enhance the training of quantum beam researchers through online classes and practical training at the facility and maximize the results of industrial applications through stronger collaboration among industry, academia, and the facility.



Chemistry is Reuniting Humanity and Nature So Tenderly

■ Prof NAKAMURA, Masaharu

Although seventy percent of the land area is forests in Japan, its forestry production accounts for only 0.05 % of the annual GDP. The production from primary industries reaches merely over 1 % even when combining agriculture, forestry, and fishery ones. Today, these primary industries, possessing various social values other than economics, face a challenging situation in Japan.

Nakamura Laboratory at International Research Center for Elements Science (IRCELS) in ICR has engaged in woody biomass molecular transformation to promote social innovation through cooperation between the primary and the chemical industries. The researchers initiated the endeavor “Exploration of Organic Synthetic Reactions Aimed at Utilizing Bio-renewable Carbon Resources” started with Prof. Takashi Watanabe of Research Institute for Sustainable Humanosphere under the support of Grant-in-Aid for Exploratory Research, Institute of Sustainable Science, Kyoto University, in 2006.

On October 8 (“Tree” Day), 2021, Kyoto University and Daicel Corporation have signed a comprehensive cooperation agreement, a comprehensive research collaboration agreement among the five departments of Kyoto university and Daicel’s research center. At the same time, “Biomass Product Tree Industry-Academia Collaborative Research Laboratory,” the industry-academia collaborative research center, was established on the Uji campus. The purpose of this collaboration is to contribute to the renovation of forests, rivers, oceans, rural areas, and cities in Japan and to realize a carbon-recycling society in good harmony with nature by creating a new industry, which transforms biomass into functional materials and chemicals. The collaborative research laboratory, a new style joint laboratory of the Institute for Chemical Research, Research Institute for Sustainable Humanosphere, Institute of Advanced Energy, and Daicel, connects academic fields, the industrial world, and the local communities.

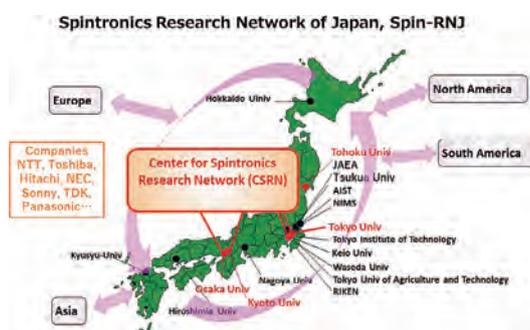
Nakamura group envisages that the comprehensive industry-academia joint research system will firmly spur “Chemistry Brighten Future (CBF).”



Introduction of Center for Spintronics Research Network, Kyoto University

■ Prof ONO, Teruo

The research community in the field of spintronics in Japan applied for the “Master Plan 2014” of the Science Council of Japan and was selected from a large number of applications (224 in all). In addition, the Ministry of Education, Culture, Sports, Science and Technology (MEXT) reviewed 27 proposals for this Master Plan, and 10 of them, including the proposal in the field of spintronics, were selected for the “Roadmap 2014—Major Projects for Academic Research”. In this project, the “Center for Spintronics Research Network (CSRN)” has been established at the hub universities (Tohoku University, the University of Tokyo, Keio University, and Osaka University) to connect major universities, national laboratories, related companies, and other leading research institutions in Japan. On the occasion of reselection for inclusion in “Master Plan 2020” and “Roadmap 2020”, the CSRN was also established in the Institute for Chemical Research, Kyoto University to strengthen the international collaboration along with the other four core universities. By linking major universities, national research institutes, related companies, and other leading research institutes in Japan, the CSRN works to enhance Japan’s research capabilities and industrial competitiveness, to bring about technological innovation, and to foster the next generation of researchers and engineers.



CONTENTS

Preface	iii
ICR News 2021	iv
ORGANIZATION	1
TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES	3
Division of Synthetic Chemistry	
Organoelement Chemistry	4
Structural Organic Chemistry	6
Synthetic Organic Chemistry	8
Advanced Inorganic Synthesis	10
Division of Materials Chemistry	
Chemistry of Polymer Materials	12
Polymer Controlled Synthesis	14
Inorganic Photonics Materials	16
Nanospintronics	18
Division of Biochemistry	
Biofunctional Design-Chemistry	20
Chemistry of Molecular Biocatalysts	22
Molecular Biology	24
Chemical Biology	26
Division of Environmental Chemistry	
Molecular Materials Chemistry	28
Hydrospheric Environment Analytical Chemistry	30
Chemistry for Functionalized Surfaces	32
Molecular Microbial Science	34
Division of Multidisciplinary Chemistry	
Polymer Materials Science	36
Molecular Rheology	38
Molecular Aggregation Analysis	40
Advanced Research Center for Beam Science	
Particle Beam Science	42
Laser Matter Interaction Science	44
Electron Microscopy and Crystal Chemistry	46
Atomic and Molecular Structures	48

International Research Center for Elements Science	
Synthetic Organotransformation	50
Advanced Solid State Chemistry	52
Organometallic Chemistry	54
Nanophotonics	56
Bioinformatics Center	
Chemical Life Science	58
Mathematical Bioinformatics	60
Bio-knowledge Engineering	62
HAKUBI RESEARCHERS' ACTIVITIES IN ICR	65
ACTIVITIES OF INTERNATIONAL JOINT USAGE/RESEARCH CENTER	67
iJURC Cooperative Research Subjects 2021	68
iJURC Publications (Selected Examples)	74
VISITING PROFESSORS' ACTIVITIES IN ICR	75
PERSONAL	77
Retirement	78
Awards	80
Paper Awards	83
Poster Awards	84
Obituary	85
PUBLICATIONS	88
INTERNATIONAL RESEARCH COLLABORATIONS	103
SELECTED GRANTS	105
THESES	112
THE 121ST ICR ANNUAL SYMPOSIUM	116
SEMINARS	119
MEETINGS AND SYMPOSIA	120
INDEX	121
NAME INDEX	122
KEYWORD INDEX	125

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



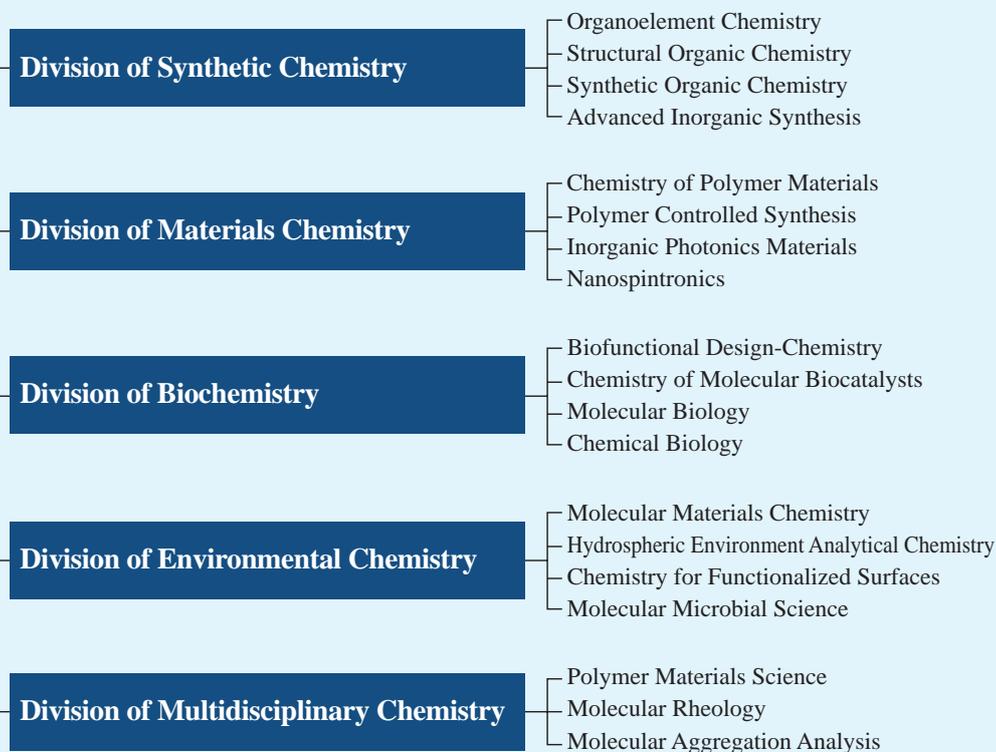
ORGANIZATION

Institute for Chemical Research

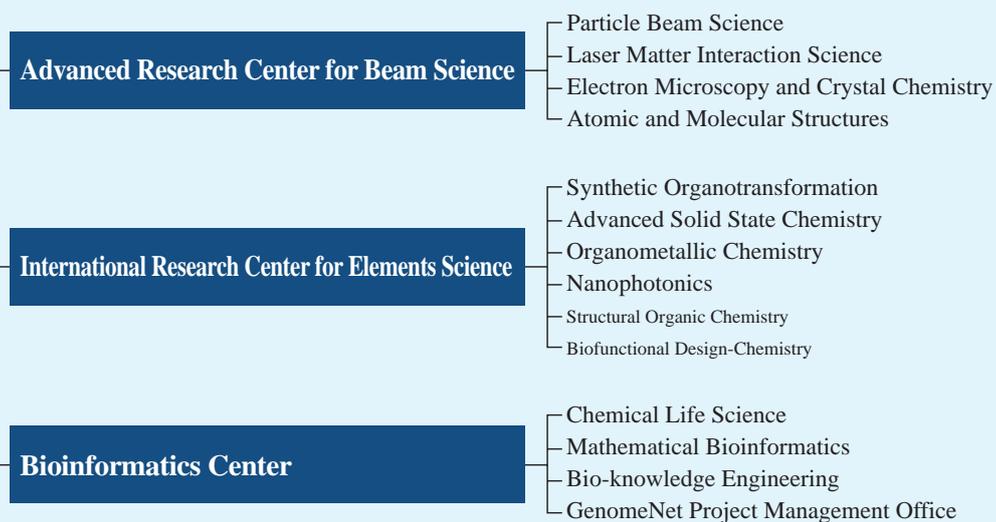
5 Divisions and 3 Centers

Laboratories

Research Divisions

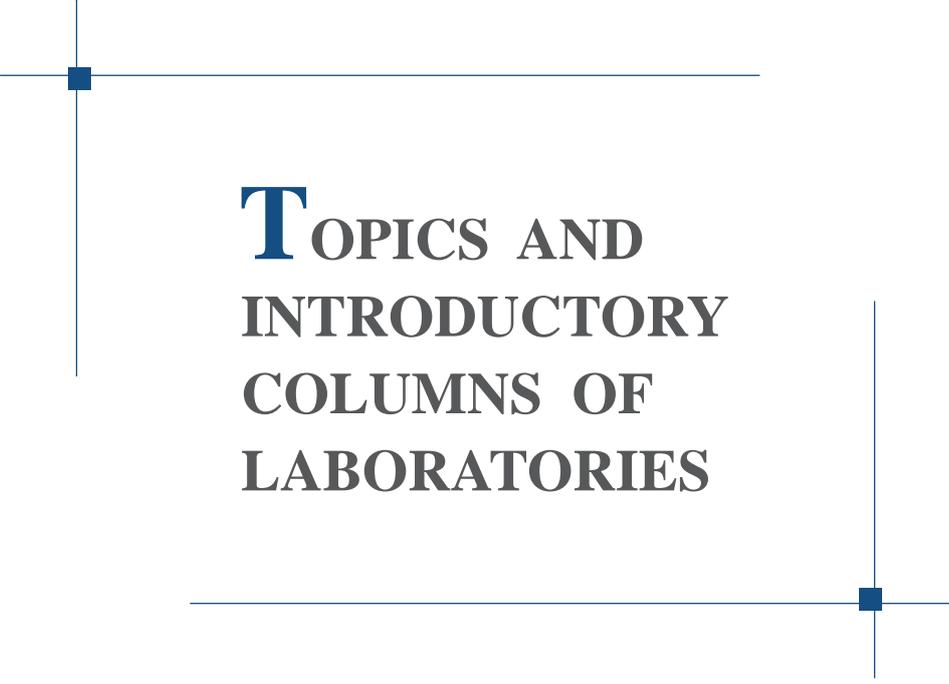


Research Centers



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

TOKITOH, Norihiro
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Assoc Prof

MIZUHATA, Yoshiyuki
(D Sc)



Assist Prof

YUKIMOTO, Mariko
(D Sc)



Techn Staff*

HIRANO, Toshiko

*Re-employed Staff

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TSUJI, Shingo (D3)

GARCIA, Julius (D2)

YANG, Yi (D1)

HONJO, Kazuma (M2)

SASAYAMA, Ryuto (M2)

KANDA, Kazuaki (M2)

SUITO, Taisuke (M2)

IJICHI, Wataru (M1)

UCHIDA, Daichi (M1)

NAKANISHI, Taiki (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



Recent Selected Publications

Yanagisawa, T.; Mizuhata, Y.; Tokitoh, N., A Novel Reactivity of Phosphanylaluminum (>P–Al<): Reversible Addition of a Saturated Interelement Bond to Olefins, *Chem. Eur. J.*, **27**, 11273–11278 (2021).

Iwai, K.; Mizuhata, Y.; Tokitoh, N., Alkali-Metal-Ion-Centered Sandwich Structures of 4-Bromophenyl[Tris(Pentafluorophenyl)]Borates and Their Synthetic Utility, *Organometallics*, **40**, 570–577 (2021).

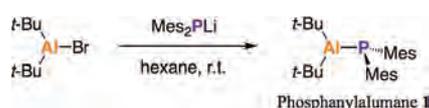
Yanagisawa, T.; Mizuhata, Y.; Tokitoh, N., Additive-Free Conversion of Internal Alkynes by Phosphanylaluminas: Production of Phosphorus/Aluminum Frustrated Lewis Pairs, *ChemPlusChem*, **85**, 933–942 (2020).

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

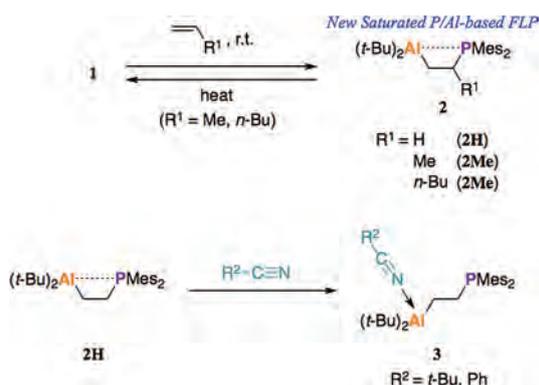
Mizuhata, Y.; Fujimori, S.; Sasamori, T.; Tokitoh, N., Germanbenzylpotassium: A Germanium Analogue of a Phenyl Anion, *Angew. Chem. Int. Ed.*, **56**, 4588–4592 (2017).

A Novel Reactivity of Phosphanylaluminum

The bonding between group 13 (E) and group 15 (Pn) elements formulated as R_2E-PnR_2 have attracted much attention due to their relationship, including the vacant p orbital on E and the lone-pair electrons on Pn. In this study, we have reported synthesis and reaction of novel λ^3, λ^3 -phosphanylaluminum **1**, Al–P single-bond species, by the reactions of aluminum monohalides [$(t\text{-Bu})_2\text{AlBr}$] with Mes_2PLi .



We found the reversible addition of olefins to phosphanylaluminum **1** to be the first case for single-bond compounds of main group elements. Although the substrate scopes of alkenes are limited to terminal alkenes ($R^1\text{-CH=CH}_2$) with relatively small substituents ($R^1 = \text{H, Me, and } n\text{-Bu}$), corresponding alkene adducts **2** were obtained. In the case of $R^1 = \text{Me}$ and $n\text{-Bu}$, the P–Al bond of the alkene adducts (**2Me** and **2Bu**) was recombined accompanied by the liberation of the corresponding alkene on heating. On the other hand, ethylene was not liberated from **2H** even on heating. We demonstrated the reactivity of **2H** as a new C2 vicinal P/Al-based FLP. In the reaction of **2H** with nitriles, nitriles were coordinated to Al as linear LBs with retention of the ethylene bridge, like the case of the P/B system.

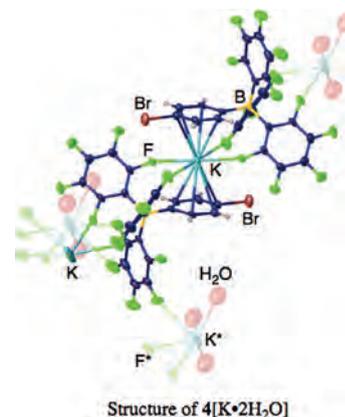
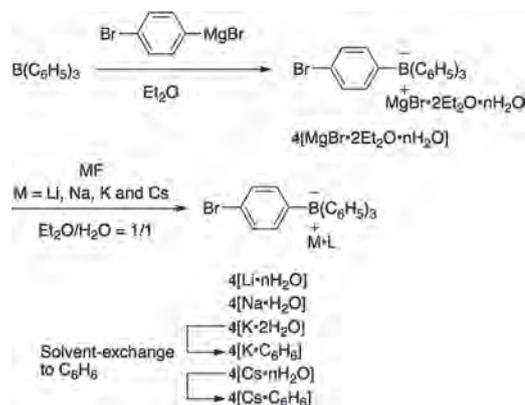


Alkali-metal-ion-centered Sandwich Structures of 4-Bromophenyl[tris(pentafluorophenyl)]borates

Fluorinated tetraarylborates (FTABs) are known as one of the best partners of reactive cations and radical cations. In addition, fascinating effects of ionic substituents have

recently gathered much attention from organic chemists. We newly designed alkali-metal 4-bromophenyl[tris(pentafluorophenyl)]borates **4**[M·L] ($M = \text{Li, Na, K, Cs, MgBr}$; $L = \text{coordinating solvents; H}_2\text{O, C}_6\text{H}_6$) as synthetic units to explore reactive cations as zwitterionic compounds.

The single-crystal X-ray diffraction analysis revealed their unique sandwich structures: that is, the bimolecular-associated sandwich structures for **4**[Na·H₂O] and **4**[K·2H₂O], the sandwich structure with C₆H₆ for **4**[K·C₆H₆], and the benzene-caged structure for **4**[Cs·2C₆H₆]. The key factor in constructing their sandwich structures was found to be the presence of coordinative *o*-fluoro groups and a π -electron-donating *p*-phenylene moiety, which form a cation-capturing pocket. Moreover, the ion radius of the counteranion was found to be a crucial factor. Remarkably, a larger cesium ion could be captured in the pocket to form a benzene-caged structure, while smaller counteranion salts **4**[MgBr·2Et₂O·*n*H₂O] and **4**[Li·*n*H₂O] could not form specific aggregates. The results of variable-temperature ¹⁹F NMR and DART-MS measurements suggested the retainment of the sandwich structures even in nonpolar solvents. The cation-capturing ability of the FTAB unit investigated in this work could be applied to the chemistry of supramolecular systems and organocatalyses.



Division of Synthetic Chemistry

– Structural Organic Chemistry –

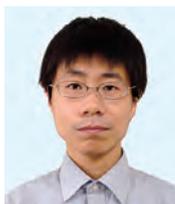
<https://www.scl.kyoto-u.ac.jp/~kouzou/en/index.html>



Prof
MURATA, Yasujiro
(D Eng)



Assoc Prof
HIROSE, Takashi
(D Eng)



Assist Prof
HASHIKAWA, Yoshifumi
(D Eng)



PD
ZHANG, Sheng
(Ph D)

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HUANG, Guanglin (D3)
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ZHANG, Zheng (D1)
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ZHU, Xiaotan (M2)
GU, Jiajian (M2)
MIYAKE, Yuya (M1)
SADAI, Shumpei (M1)

ZENG, Yuting (M1)
LIU, Zhibo (M1)
OKUSHIMA, Ryota (UG)
FUJIKAWA, Nana (UG)

HIRA, Shota (UG)

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



Recent Selected Publications

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.*, **60**, 2866-2870 (2021).

Hashikawa, Y.; Kizaki, K.; Murata, Y., Pressure-Induced Annulative Orifice Closure of a Cage-Opened C_{60} Derivative, *Chem. Commun.*, **57**, 5322-5325 (2021).

Zhang, S.; Hashikawa, Y.; Murata, Y., Cage-Expansion of Fullerenes, *J. Am. Chem. Soc.*, **143**, 12450-12454 (2021).

Hashikawa, Y.; Sadai, S.; Murata, Y., Reductive Decarbonylation of a Cage-Opened C_{60} Derivative, *Org. Lett.*, **23**, 9495-9499 (2021).

Hashikawa, Y.; Murata, Y., Synthesis and Oligomerization of $CpM(CO)_2$, *ACS Omega*, **6**, 34137-34141 (2021).

Kubo, H.; Hirose, T.; Nakashima, T.; Kawai, T.; Hasegawa, J.-Y.; Matsuda, K., Tuning Transition Electric and Magnetic Dipole Moments: [7] Helicenes Showing Intense Circularly Polarized Luminescence, *J. Phys. Chem. Lett.*, **12**, 686-695 (2021).

Cage-Expansion of Fullerenes

Despite the first proposal on the cage inflation of fullerenes in 1991, the chemical expansion of fullerenes has been still a formidable challenge. Herein, we provide an efficient methodology to expand [60] and [70] fullerene cages by the inclusion of totally C5N unit, giving nitrogen-containing closed structures as C₆₅N and C₇₅N with double fused heptagons. This method consists of two steps commenced with the construction of an opening by the reaction with triazine as a C3N source, followed by the cage reformation using *N*-phenylmaleimide as a C2 source. We also synthesized endohedral cages, demonstrating that the encapsulated H₂O molecule inside the C₇₅N cage prefers the orientation which maximizes the intramolecular interaction with the carbon wall. Additionally, we revealed the existence of a through-space magnetic dipolar interaction between the encapsulated H₂ molecule and the embedded N-atom.

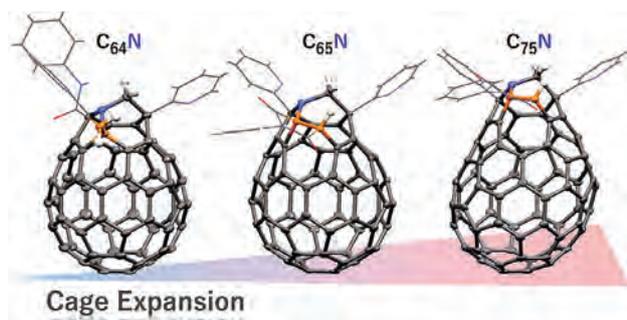


Figure 1. Cage-expanded fullerenes.

Synthesis and Oligomerization of CpM(CO)₂

We showcase efficient synthetic protocols of cyclopentadienyl metal dicarbonyl, CpM(CO)₂ (M = Rh and Ir). Reflecting the relativistic effect, the ¹H and ¹³C signals of the Cp ring in CpIr(CO)₂ were upfield shifted when compared with the Rh analogue. A missing dinuclear complex, (CpIr)₂(μ-CO)(CO)₂, was spontaneously generated together with [CpIr(CO)]₃ by the loss of CO. The crystallographic analyses unambiguously determined their unique structures with one and three Ir–Ir bonds, respectively.

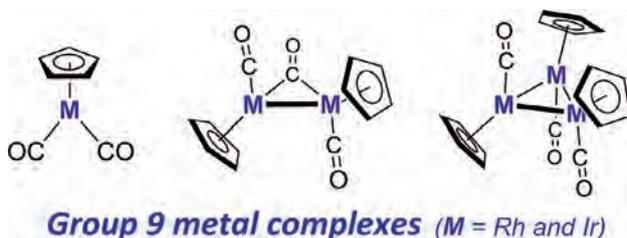


Figure 2. Cyclopentadienyl group 9 metal carbonyl complexes.

Tuning Transition Electric and Magnetic Dipole Moments: [7]Helicenes Showing Intense Circularly Polarized Luminescence

Helicenes are promising candidates for chiral optoelectronic materials, however, the emission intensity of unsubstituted helicenes is very weak ($\Phi_f < 0.05$) due to a small oscillator strength for the S₁→S₀ transition. In this work, we designed the S₁→S₀ transition of [7]helicene derivatives so that it has a large transition magnetic dipole moment (TMDM) and is partially symmetry-allowed. A [7]helicene derivative thus designed showed a large fluorescence emission rate ($k_f = 0.02 \text{ ns}^{-1}$) and a large TMDM for the S₁→S₀ transition ($|m| = 2.37 \times 10^{-20} \text{ erg} \cdot \text{Gauss}^{-1}$), which are more than 10 times greater than those of unsubstituted [7]helicene ($k_f = 0.001 \text{ ns}^{-1}$, $|m| = 0.045 \times 10^{-20} \text{ erg} \cdot \text{Gauss}^{-1}$). As a result, we achieved the [7]helicene derivative whose dissymmetry factor of CPL and fluorescence quantum yield were both high ($|g_{\text{CPL}}| = 1.3 \times 10^{-2}$, $\Phi_f = 0.17$) in the solution phase.

Design of **Magnetically-Allowed** S₁→S₀ Transitions

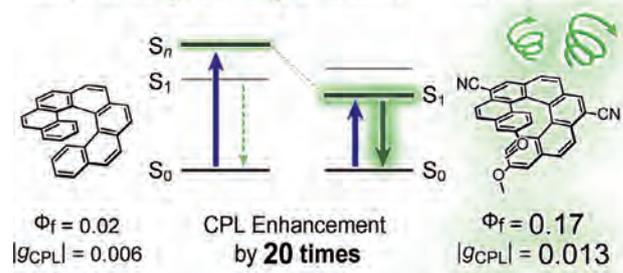


Figure 3. A design of emissive [7]helicene with large dissymmetry factor of CPL.

Division of Synthetic Chemistry

– Synthetic Organic Chemistry –

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Students

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FUJIMURA, Kouki (D1)
TANIGAKI, Yusuke (M2)

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) organocatalytic site-selective transformation of multi-functionalized molecules, 2) dirhodium-catalyzed site-selective C-H functionalization, 3) asymmetric induction in transformation of compounds with molecular chirality, 4) total synthesis of glycoside-based natural product based on sequential site-selective functionalization.

KEYWORDS

Site-Selective Functionalization
Molecular Recognition
Molecular Catalyst
Sugar
Natural Product

Recent Selected Publications

- Shibayama, H.; Ueda, Y.; Tanaka, T.; Kawabata, T., Seven-Step Stereodivergent Total Synthesis of Punicafolin and Macaranganin, *J. Am. Chem. Soc.*, **143**, 1428-1434 (2021).
- 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).
- Chen, G.; Arai, K.; Morisaki, K.; Kawabata, T.; Ueda, Y., Dirhodium-Catalyzed Chemo- and Site-Selective C-H Amination of *N,N*-Dialkylanilines, *Synlett*, **32**, 728-732 (2021).
- Takeuchi, H.; Fujimori, Y.; Ueda, Y.; Shibayama, H.; Nagaishi, M.; Yoshimura, T.; Sasamori, T.; Tokitoh, N.; Furuta, T.; Kawabata, T., Solvent-Dependent Mechanism and Stereochemistry of Mitsunobu Glycosylation with Unprotected Pyranoses, *Org. Lett.*, **22**, 4754-4759 (2020).
- Ninomiya, R.; Arai, K.; Chen, G.; Morisaki, K.; Kawabata, T.; Ueda, Y., β -Silicon-Effect-Promoted Intermolecular Site-Selective C(sp³)-H Amination with Dirhodium Nitrenes, *Chem. Commun.*, **56**, 5759-5762 (2020).
- Yanagi, M.; Ueda, Y.; Ninomiya, R.; Imayoshi, A.; Furuta, T.; Mishihiro, K.; Kawabata, T., Synthesis of 4-Deoxy Pyranosides via Catalyst-Controlled Site-Selective Toluoylation of Abundant Sugars, *Org. Lett.*, **21**, 5006-5009 (2019).
- Arai, K.; Ueda, Y.; Morisaki, K.; Furuta, T.; Sasamori, T.; Tokitoh, N.; Kawabata, T., Intermolecular Chemo- and Regioselective Aromatic C-H Amination of Alkoxyarenes Promoted by Rhodium Nitrenoids, *Chem. Commun.*, **54**, 2264-2267 (2018).
- Yanagi, M.; Imayoshi, A.; Ueda, Y.; Furuta, T.; Kawabata, T., Carboxylate Anions Accelerate Pyrrolidinopyridine (PPy)-Catalyzed Acylation: Catalytic Site-Selective Acylation of a Carbohydrate in Situ Counteranion Exchange, *Org. Lett.*, **19**, 3099-3102 (2017).

Seven-step Stereodivergent Total Syntheses of Punicafolin and Macaranganin

Ellagitannins constitute one of the major classes of hydrolysable tannins and more than 500 natural products have been structurally characterized. Punicafolin (**1**) and macaranganin (**2**), natural glycosides of an ellagitannins family, are characterized by a 3,6-hexahydroxydiphenoyl (HHDP) group bridged between C(3)-OH and C(6)-OH of the glucose core. (Figure 1). They are stereoisomeric to each other concerning the chiral axis of the HHDP moiety and show different biological activities depending on the chirality of the HHDP group. Although stereodivergent synthesis of the HHDP groups is desirable for their straightforward total syntheses, construction of the 3,6-HHDP group has been a synthetic challenge because a less stable axial-rich 1C_4 conformer of the pyranose ring is required for the formation. We achieved the first total syntheses of **1** and **2** in 7 steps, respectively from D-glucose. The prominent features of the synthesis are; (1) sequential site-selective introduction of the adequate galloyl groups into unprotected D-glucose by a catalyst-controlled manner employing originally developed organocatalysts **C1** and **C2**, and (2) stereodivergent construction of the 3,6-HHDP bridge by oxidative phenol coupling of a common intermediate via a ring flipping process of the glucose core. Because no protective groups were used for glucose throughout the process, extremely short-step total syntheses were achieved.

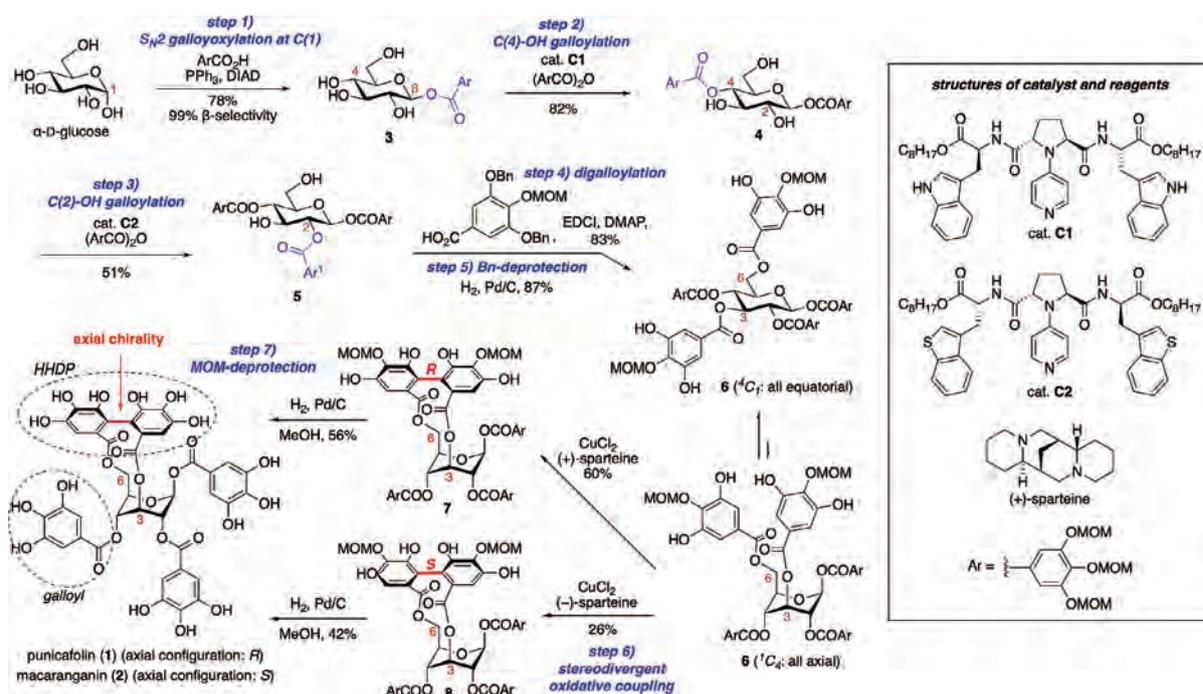


Figure 1. Total synthesis of punicafolin and macaranganin.

Dirhodium-catalyzed Chemo- and Site-Selective C-H Amination of Dialkylanilines

Development of methods for the construction of C-N bonds is still of great synthetic importance in current synthetic organic chemistry because C-N bonds are ubiquitously involved in functional materials and bioactive molecules. Especially, direct C-N bond formation through C-H bond cleavage represents an attractive and efficient access to such functional molecules. We recently reported a method for dirhodium-catalyzed C(sp³)-H amidation of *N,N*-dimethylanilines (Figure 2). Chemo- and site-selective C(sp³)-H amidation of *N*-methyl group proceeded exclusively in the presence of C(sp²)-H bonds of the electron-rich aromatic ring and secondary, tertiary, and benzylic C(sp³)-H bonds α to a nitrogen atom. The protocol was successfully applied to a two-step demethylation process of a *N*-methylaniline derivative.

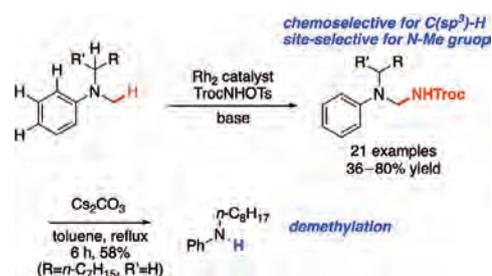


Figure 2. Chemo- and site-selective C-H amination and application to de-methylation.

Division of Synthetic Chemistry

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*New Research Field
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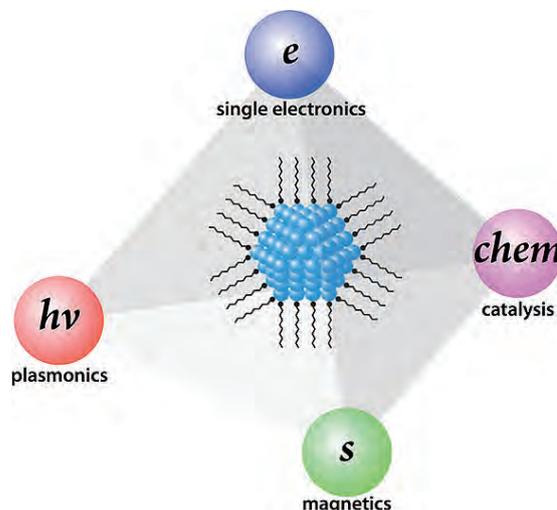
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Scope of Research

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



Recent Selected Publications

Saruyama M.; Sato R.; Teranishi T., Transformations of Ionic Nanocrystals via Full and Partial Ion Exchange Reactions, *Acc. Chem. Res.*, **54**, 765-775 (2021).

Li Z.; Saruyama M.; Asaka T.; Tatetsu Y.; Teranishi T., Determinants of Crystal Structure Transformation of Ionic Nanocrystals in Cation Exchange Reactions, *Science*, **373**, 332-337 (2021).

Novel Cu–Ni Bimetallic Selenide Nanocrystals Formed via Cation Exchange Reaction for Water Oxidation Catalysis

Controlling composition and nanostructure of electrocatalysts is important for dramatic improvement of the catalytic performance. The cation exchange reaction of nanocrystals (NCs) has been considered as facile way to provide unusual crystal structures and sophisticated functional nanostructures that cannot be achieved by conventional direct synthetic procedure. We demonstrated the cation exchange-derived formation of metastable spinel Ni_3Se_4 NCs from berzelianite Cu_{2-x}Se NCs, and the formation of novel Cu–Ni selenide NCs as active oxygen evolution reaction (OER) catalysts. A rare spinel Ni_3Se_4 phase was formed because the face-centered cubic (fcc) Se^{2-} sublattice in Cu_{2-x}Se NCs was kinetically retained throughout the cation exchange process (Figure 1a). Partial cation exchange reaction by tuning the Ni/Cu mole ratio led to the formation of Janus-type $\text{Cu}_{2-x}\text{Se}/\text{Ni}_3\text{Se}_4$ NCs, exhibiting remarkable catalytic activities in the OER with small overpotentials of 230 mV at 10 mA cm^{-2} in 0.1 M KOH. These results imply that the cation exchange reaction could have huge potential for the creation of novel heterostructured NCs showing superior electrocatalytic performance.

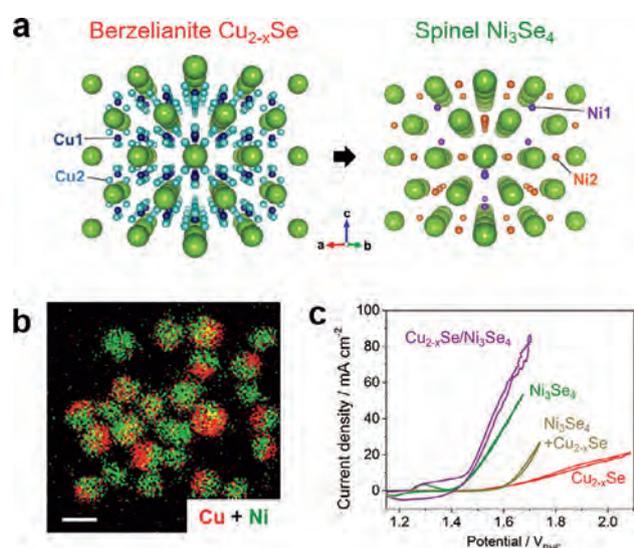


Figure 1. (a) Retention of fcc Se lattice of Cu_{2-x}Se NCs during Cu^+ to Ni^{2+} cation exchange. (b) STEM-EDS mapping of $\text{Cu}_{2-x}\text{Se}/\text{Ni}_3\text{Se}_4$ NCs formed via partial cation exchange. (c) CVs of NCs in 0.1 M KOH.

Revealing the Determinants of Crystal Structure Transformation of Ionic Nanocrystals in Cation Exchange Reactions

Ionic NCs have been widely utilized as photo-functional materials, whose properties are determined by the constituent elements and crystal structures. Cation exchange reaction can easily modulate the composition of ionic NCs to prepare a variety of functional nanomaterials. However, it has been believed that cation exchange hardly changes the crystal structure of parent ionic NCs. We applied the cation exchange reaction to hexagonal-prism-shaped $\text{Cu}_{1.8}\text{S}$ NCs with 16 kinds of height and width using Co^{2+} . It was discovered that crystal system of resultant CoS_x NCs depends on the height of parent $\text{Cu}_{1.8}\text{S}$ NCs, in which the original hexagonal-close-packed (hcp) crystal system of $\text{Cu}_{1.8}\text{S}$ NCs with thicker or thinner than about 10 nm yielded cubic-close-packed (ccp) Co_9S_8 or hcp CoS NCs, respectively (Figure 2). The ab-initio calculation revealed the surface energy of side surface is larger than that of basal plane in hcp CoS , suggesting unfavored large side surface area of thick hcp CoS NCs induced the phase transformation into more stable ccp Co_9S_8 . Other incoming cations (Mn^{2+} , Zn^{2+} , and Ni^{2+}) modulated the phase transformation trend in cation exchange reactions by various means, such as volume, thermodynamic stability, and coordination environment. This discovery could lead to the phase control of ionic NCs under mild condition, which enables the synthesis of unexplored functional ionic nanomaterials.

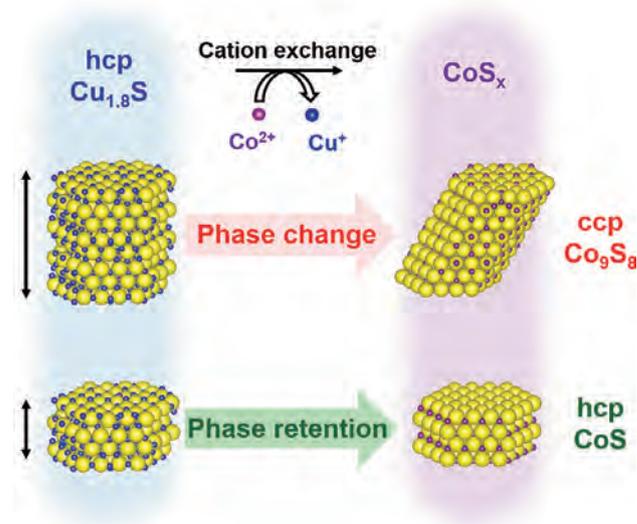


Figure 2. Height of hexagonal-prism $\text{Cu}_{1.8}\text{S}$ NCs determines the crystal structure of products after Co^{2+} cation exchange.

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Scope of Research

We perform kinetic and mechanistic analyses toward understanding chemical and physicochemical reactions occurring in polymerization systems and better routes for synthesis of well-defined polymers. In particular, new well-defined polymers or polymer assemblies are prepared by living polymerization techniques, and their structure–properties relationships are precisely analyzed. Projects in progress include: 1) kinetics and mechanisms of living radical polymerization (LRP); 2) synthesis of new polymeric materials by living polymerizations and their structure/properties studies; and 3) synthesis, properties, and applications of concentrated polymer brushes (CPB).

KEYWORDS

Precision Polymerization Living Radical Polymerization
Polymer Brush Tribology
Hybrid Materials



Recent Selected Publications

- Sakakibara, K.; Ishida, H.; Kinose, Y.; Tsujii, Y., Regioselective Synthesis of Cellulosic Janus Bottlebrushes with Polystyrene and Poly (ϵ -Caprolactone) Side Chains and Their Solid-State Microphase Separation, *Cellulose*, **28**, 6857-6868 (2021).
- Kinose, Y.; Sakakibara, K.; Sato, O.; Tsujii, Y., Near-Zero Azimuthal Anchoring of Liquid Crystals Assisted by Viscoelastic Bottlebrush Polymers, *ACS Appl. Mater.*, **3**, 2618-2625 (2021).
- Sakakibara, K.; Maeda, K.; Yoshikawa, C.; Tsujii, Y., Water Lubricating and Biocompatible Films of Bacterial Cellulose Nanofibers Surface-Modified with Densely Grafted, Concentrated Polymer Brushes, *ACS Appl. Nano Mater.*, **4**, 1503-1511 (2021).
- Maguire, S. M.; Krook, N. M.; Kulshreshtha, A.; Bilchak, C. R.; Brosnan, R.; Pana, A.-M.; Rannou, P.; Maréchal, M.; Ohno, K.; Jayaraman, A.; Composto, R. J., Interfacial Compatibilization in Ternary Polymer Nanocomposites: Comparing Theory and Experiments, *Macromolecules.*, **54**, 797-811 (2021).
- Maguire, S. M.; Boyle, M. J.; Bilchak, C. R.; Demaree, J. D.; Keller, A. W.; Krook, N. M.; Ohno, K.; Kagan, C. R.; Murray, C. B.; Rannou, P.; Composto, R. J., Grafted Nanoparticle Surface Wetting during Phase Separation in Polymer Nanocomposite Films, *ACS Appl. Mater. Interfaces.*, **13**, 37628-37637 (2021).

Synthesis of Cellulosic Janus Bottlebrushes with Polystyrene and Poly(ϵ -Caprolactone) Side Chains

Graft polymer with dense side chains is called bottlebrush. A type of bottlebrush (BB) possessing different types of side chains (Janus BB) attracts attentions as a building block for high-order structures because immiscible side chains could undergo microphase separation, where the main chain is located at the interface.

We have successfully synthesized a novel cellulosic Janus BB with polystyrene (PS) and poly(ϵ -caprolactone) (PCL) as side chains (Figure 1a). The two types of side chains were regioselectively grafted by “grafting-from” (for PCL at *O*-2,3 positions) and “grafting-to” (PS at *O*-6 position) techniques with the aid of a *p*-methoxytrityl protecting group. The degree of substitution (DS) of PCL (degree of polymerization (DP) = 100) was estimated to be 1.5, and that of PS was estimated to be 0.64–0.84 depending on its chain length (DP = 38, 90 or 158). As for the high-order structure of cellulosic Janus BB, annealed samples were observed by transmission electron microscopy (TEM) (Figure 1b). The cellulosic Janus BB (PS/PCL = 50:50 v/v) was revealed to form a lamellar microdomain structure with three layers. These layers were attributed to amorphous PCL, crystalline PCL, and amorphous PS layers, indicating that the main chain of the BB (cellulose) was located at the interface between amorphous PS and amorphous PCL layers and hindered the crystallization of PCL segments near the main chain. It is expected that further tuning of the structural parameters of cellulosic Janus BB could lead to chiral or helical high-order structures, bringing intriguing functionalities.

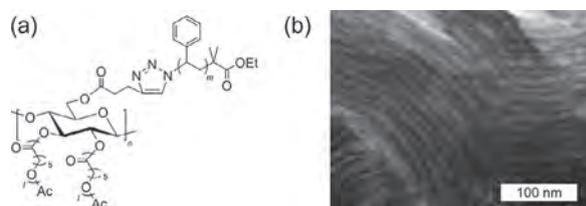


Figure 1. (a) Chemical structure of cellulosic BB and (b) TEM image of its annealed bulk film (PCL: DS = 1.5, DP = 100; PS: DS = 0.75, DP = 90).

Relaxation Behavior of Side Chain and Anchoring Property of Liquid Crystal on Cross-Linked Bottlebrush Polymer Film

The liquid crystals (LCs) in bulk can be aligned by external fields such as electric and magnetic fields, whereas the change in the direction of LCs near a surface is restricted

by the interaction between LCs and the surface, which is known as the anchoring effect. In contrast to a strong anchoring case, it is difficult to fabricate an extremely weak anchoring (zero anchoring) surface with sufficient stability. It had been reported that the concentrated polymer brush and cross-linked BB (Figure 2a) comprised of poly(hexyl methacrylate) (PHMA) provided a zero-azimuthal anchoring property even at low temperature.

We have investigated the anchoring mechanism of LCs on a brush structure consisting of cross-linked films of PHMA BBs (Figure 2b). The azimuthal anchoring coefficient A_2 was estimated from the voltage–transmittance curves and found to decrease with increasing temperature in a certain temperature range (Figure 3a). Then, the rheological measurement for the mixture of BB and LC was carried out to discuss the relaxation behavior of the side chain of BB (Figure 3b). As a result, the characteristic temperature of the side-chain motion corresponded to the above-mentioned, A_2 -decreasing temperature range (Figure 3a). This was also the case with the poly(ethyl methacrylate) (PEMA) BB system. Consequently, it was concluded that the weak anchoring of LCs on a polymer-brush-coated surface was attributed to the polymer-chain dynamics and that the A_2 value could be lowered by the brush structure achieving higher mobility as well as the brush chemistry promoting the swelling in LCs.

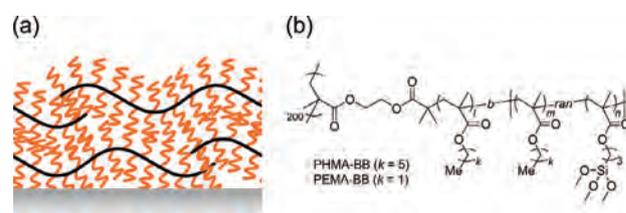


Figure 2. Schematic illustration of cross-linked BB film (a) and chemical structure of BB with cross-linking moiety (b).

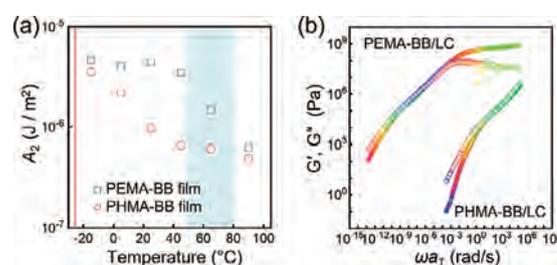


Figure 3. The relation between A_2 and temperature; the red line and blue shade indicate the characteristic temperatures of the relaxation of side chains for PHMA and PEMA BB films, respectively. (b) Master curves of G' (filled circles) and G'' (open circles) for mixtures of PHMA-BB and PEMA-BB with LCs, respectively. Reprinted (adapted) with permission from Ref. No 1. Copyright 2021 American Chemical Society.

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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 Synthesis

Living Radical Polymerization

Polymer Properties

Curved π -Conjugated Molecules

Recent Selected Publications

Li, X.; Kato, T.; Nakamura, Y.; Yamago, S., The Effect of Viscosity on the Coupling and Hydrogen-Abstraction Reaction between Transient and Persistent Radicals, *Bull. Chem. Soc. Jpn.*, **94**, 966-972 (2021).

Park, B.; TosaKa, M.; Yamago, S., Crystallization of Isotactic Poly(*N,N*-diethyl acrylamide) Synthesized by Ytterbium Triflate/H₂O Catalyzed Stereoselective Radical Polymerization, *Polym. J.*, **53**, 533-538 (2021).

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).

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).

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).

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.

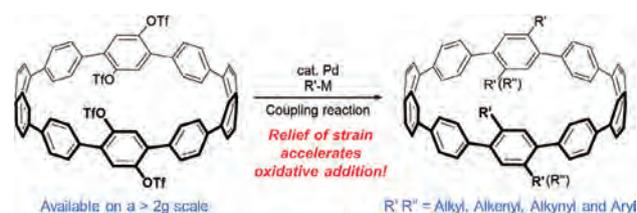


Figure 1. Synthesis of tetrasubstituted [10]cycloparaphenylene derivatives bearing alkyl, alkenyl, alkynyl and aryl substituents.

Tacticity, Molecular Weight, and Temporal Control by Lanthanide Triflate-catalyzed Stereoselective Radical Polymerization of Acrylamides with an Organotellurium Chain Transfer Agent

Polymerization of *N,N*-dimethylacrylamide, *N*-isopropylacrylamide, *N,N*-diethylacrylamide, and acrylamide while controlling both molecular weight and stereoregularity was achieved by organotellurium-mediated radical polymerization (TERP) in the presence of $Y(OTf)_3$ or $Yb(OTf)_3$ as a Lewis acid catalyst. In previous works, dual-control reactions have been limited to the synthesis of low-molecular-weight polyacrylamides. On the other hand, the current conditions could overcome this limitation. We could demonstrate the high compatibility of the TERP chain transfer agent and dormant species to the Lewis acid by nearly complete end-group fidelity. Stereoblock copolymers consisting of atactic and isotactic PDEAA blocks were also successfully synthesized. Temporal control while maintaining dual control was also accomplished by using photoactivation of organotellurium species. The effect of tacticity on the polymer structure in the gas phase was studied for the first time by ion mobility spectrometry, revealing that the collision cross section increased as the meso diad selectivity of the polyacrylamide increased.

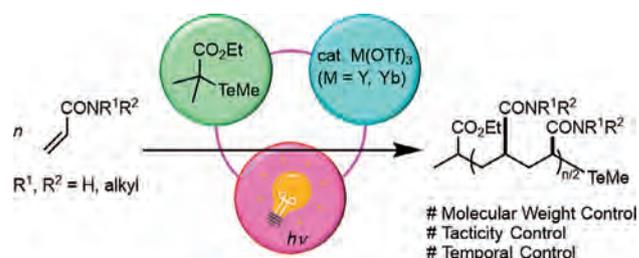


Figure 2. Polymerization of acryl amide with controlled tacticity, molecular weight, and temporal progress.

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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



Recent Selected Publications

Herbschleb, E. D.; Kato, H.; Makino, T.; Yamasaki, S.; Mizuochi, N., Ultra-High Dynamic Range Quantum Measurements Retaining Its Sensitivity, *Nat. Commun.*, **12**, 306 (2021).

Watanabe, A.; Nishikawa, T.; Kato, H.; Fujie, M.; Fujiwara, M.; Makino, T.; Yamasaki, S.; Herbschleb, E. D.; Mizuochi, N., Shallow NV Centers Augmented by Exploiting N-Type Diamond, *Carbon*, **178**, 294-300 (2021).

Kobayashi, S.; Matsuzaki, Y.; Morishita, H.; Miwa, S.; Suzuki, Y.; Fujiwara, M.; Mizuochi, N., Electrical Control for Extending of Ramsey Spin Coherence Time of Ion-Implanted NV Centers in Diamond, *Phys. Rev. Appl.*, **14**, 044033 (2020).

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.

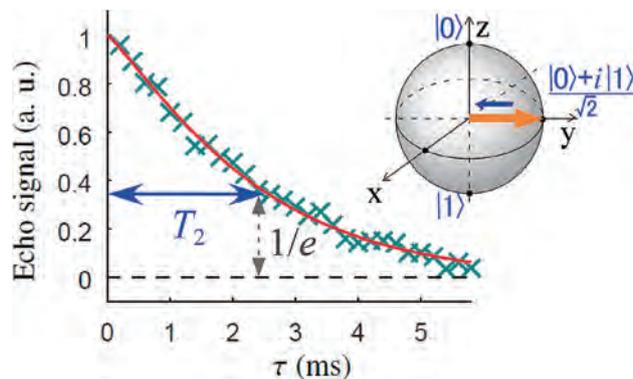


Figure 1. Echo signal of the single NV centre at room temperature. (Insert) Bloch sphere to show the coherence (superposition state).

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.

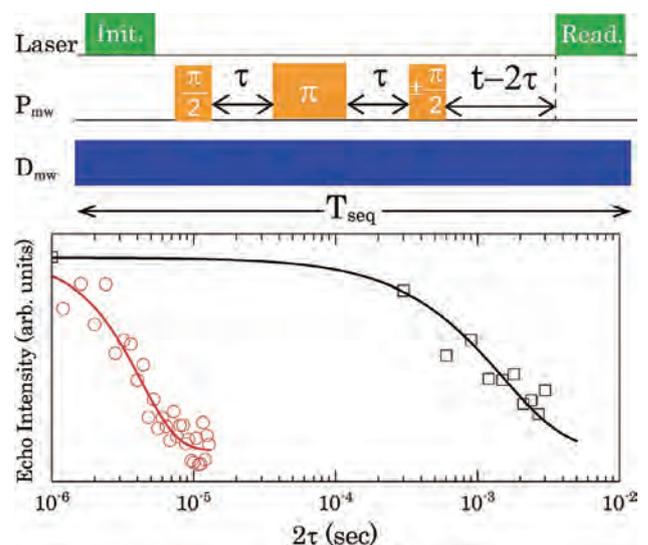


Figure 2. (Top) Pulse sequence to observe T_{2p} and T_2 with applying a phase cycle to the final $\pi/2$ pulse. (Bottom) Black and red plots show the results of T_{2p} and T_2 measurements, respectively. They are fitted by exponential decay curves described by black and red solid lines.

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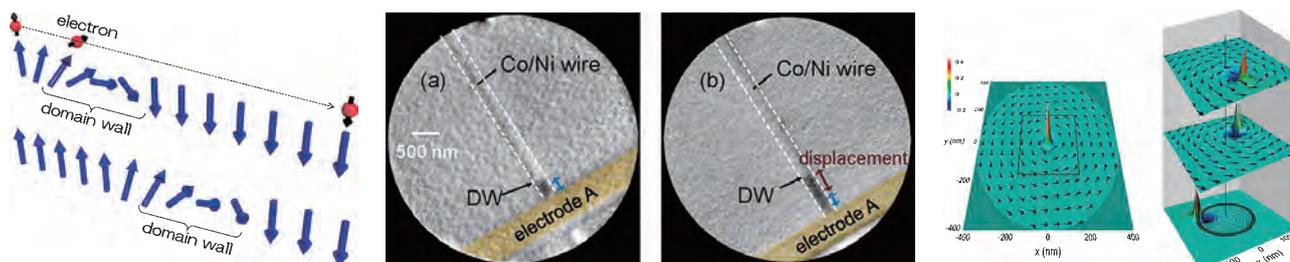
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Scope of Research

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



Recent 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).

Spin-transfer-torque-driven Magnetic Domain Wall Motion in Antiferromagnetically Coupled Ferrimagnets

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

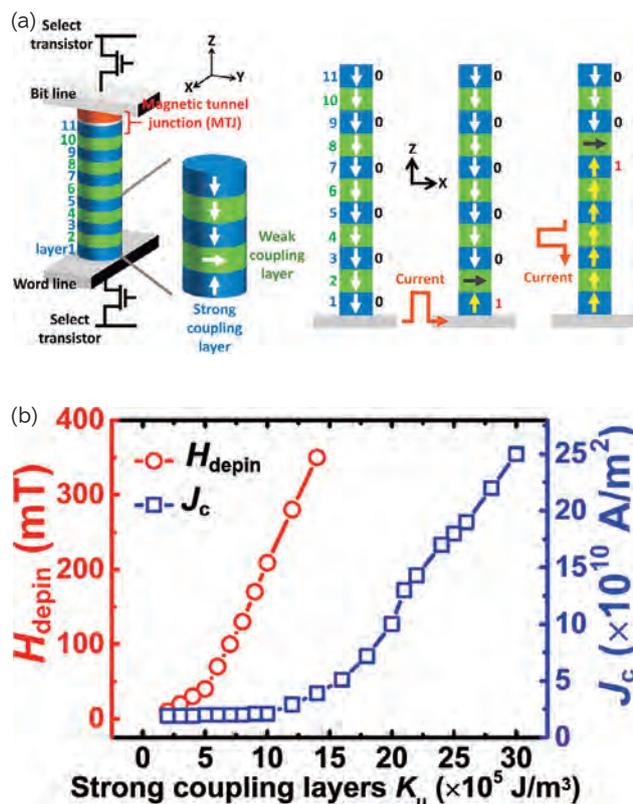


Figure 1. (a) Schematic illustration of the experimental setup. (b) The STT-induced DW velocity as a function of temperature. The dotted orange line represents the angular momentum compensation temperature T_A .

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.

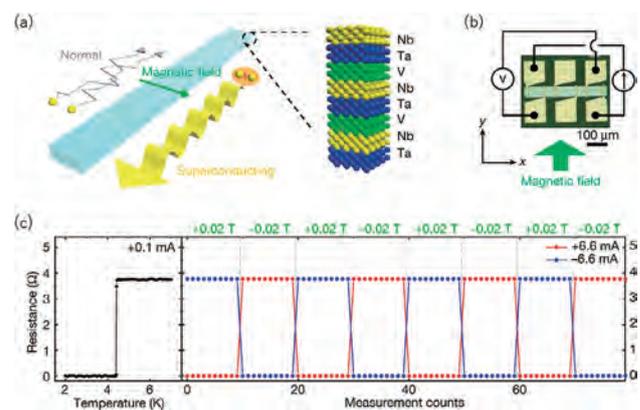


Figure 2. (a) Schematic images of the superconducting diode controlled by an external magnetic field and the artificial $[\text{Nb}/\text{V}/\text{Ta}]_n$ superlattice, in which the global inversion symmetry is broken along the direction of stacking. When the directions of the current, the magnetic field 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.

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Scope of Research

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



KEYWORDS

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

Recent Selected Publications

Iwata, T.; Hirose, H.; Sakamoto, K.; Hirai, Y.; Arafiles, J. V. V.; Akishiba, M.; Imanishi, M.; Futaki, S., Liquid Droplet Formation and Facile Cytosolic Translocation of IgG in the Presence of Attenuated Cationic Amphiphilic Lytic Peptides, *Angew. Chem. Int. Ed.*, **60**, 19804-19812 (2021).

Hirai, Y.; Hirose, H.; Imanishi, M.; Asai, T.; Futaki, S., Cytosolic Protein Delivery Using pH-Responsive, Charge-Reversible Lipid Nanoparticles, *Sci. Rep.*, **11**, 19896 (2021).

Sakamoto, K.; Michibata, J.; Hirai, Y.; Ide, A.; Ikitoh, A.; Takatani-Nakase, T.; Futaki, S., Potentiating the Membrane Interaction of an Attenuated Cationic Amphiphilic Lytic Peptide for Intracellular Protein Delivery by Anchoring with Pyrene Moiety, *Bioconjug. Chem.*, **32**, 950-957 (2021).

Arafiles, J. V. V.; Hirose, H.; Hirai, Y.; Kuriyama, M.; Sakyiamah, M. M.; Nomura, W.; Sonomura, K.; Imanishi, M.; Otaka, A.; Tamamura, H.; Futaki, S., Discovery of a Macropinocytosis-Inducing Peptide Potentiated by Medium-Mediated Intramolecular Disulfide Formation, *Angew. Chem. Int. Ed.*, **60**, 11928-11936 (2021).

Sakamoto, K.; Akishiba, M.; Iwata, T.; Murata, K.; Mizuno, S.; Kawano, K.; Imanishi, M.; Sugiyama, F.; Futaki, S., Optimizing Charge Switching in Membrane Lytic Peptides for Endosomal Release of Biomacromolecules, *Angew. Chem. Int. Ed.*, **59**, 19990-19998 (2020).

Liquid Droplet Formation and Facile Cytosolic Translocation of IgG in the Presence of Attenuated Cationic Amphiphilic Lytic Peptides

Antibodies (IgGs) have excellent antigen recognition ability and are not only used as a tool for molecular analysis in the life science field, but are also being developed as molecular targeting drugs. However, due to their large size (approximately 150 kDa) and hydrophilicity, IgGs are unable to penetrate cell membranes, making it difficult to target intracellular molecules. In our laboratory, we have developed L17E, a macromolecule delivery peptide [1]. L17E enables efficient intracellular delivery of macromolecules, including IgGs. However, to achieve effective intracellular delivery of IgGs by L17E and recognition of subcellular targets by IgGs, L17E and IgGs must be administered at high concentrations (L17E 40 μ M, IgG 0.5–1 mg/mL). In view of the application to basic research such as cell biology and clinical application, it is necessary to develop a method that enables efficient intracellular delivery of L17E and IgG at lower concentrations.

We hypothesized that increasing the local concentration of IgG and L17E in the vicinity of the membrane would be important for efficient intracellular delivery of IgG. To increase the local concentration of L17E, we prepared an L17E analogue [FcB(L17E)₃] comprised of trimerized L17E tethered with a peptide sequence having binding ability to IgG. Marked intracellular delivery of IgGs was achieved using FcB(L17E)₃ at lower peptide and IgG concentrations than with L17E. Different from our original expectation, liquid-liquid phase separation, caused by the electrostatic interaction between the FcB(L17E)₃ and the fluorescently labeled IgG, was found to be the driving force to attain the facile antibody delivery into cells (Figure 1) [2]. The results of this research are expected to serve as a basis for the development of new drug carriers based on liquid-liquid phase separation in the future.

References

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 [2] Iwata, T. *et al.*, *Angew. Chem. Int. Ed.*, **60**, 19804-19812 (2021).

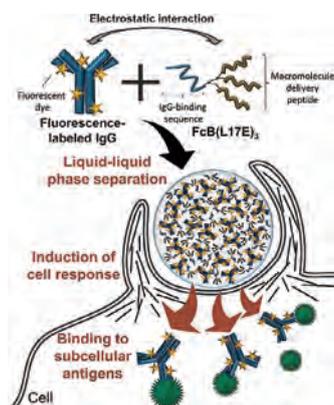


Figure 1. Proposed mechanism of action of FcB(L17E)₃.

Cytosolic Delivery of Negatively Charged Protein Using pH-responsive, Charge-reversible Lipid Nanoparticles

Proteins have attractive features as biopharmaceuticals because of their specific effects to target molecules. However, their applicability is limited to only extracellular environment because it is difficult to deliver them into the cell interior. Lipid nanoparticles (LNPs) composed with pH-responsive lipids are a promising class of intracellular delivery vehicles of negatively charged molecules like nucleic acids. In using LNPs system for protein delivery, the major challenges include: (i) formulation of LNPs with appropriate particle sizes and dispersity, (ii) efficient encapsulation of proteins into LNPs, and (iii) effective cellular internalization and cytosolic release of proteins. To develop new carrier for protein delivery, we used dioleoylglycerophosphate-diethylenediamine (DOP-DEDA), a pH-responsive, charge-reversible lipid for delivery of nucleic acids into human cancer cells [1]. A negatively charged green fluorescent protein analog with nuclear localization signal (NLS-(−30)GFP) was successfully encapsulated into DOP-DEDA-based LNPs (protein encapsulation efficiency, ~ 80 %) to yield particle diameters and polydispersity index of < 200 nm and < 0.2, respectively. Intracellular distribution of fluorescent signals of the protein was observed for up to ~ 90 % of cells treated with DOP-DEDA-based LNPs. Overall, our results indicate the facilitated endocytic uptake and endosomal escape of a negatively charged protein attained using DOP-DEDA-based LNP system.

Reference

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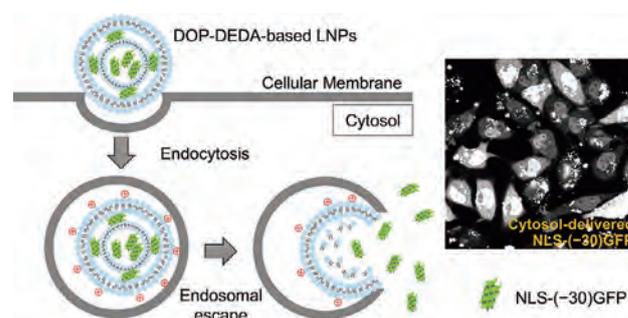


Figure 2. DOP-DEDA-based LNPs enhance intracellular and cytosolic delivery of negatively charged protein.

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Scope of Research

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

KEYWORDS

Plant Hormone
Strigolactone
Biosynthesis
Cytochrome P450
Receptor



Recent Selected Publications

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

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.

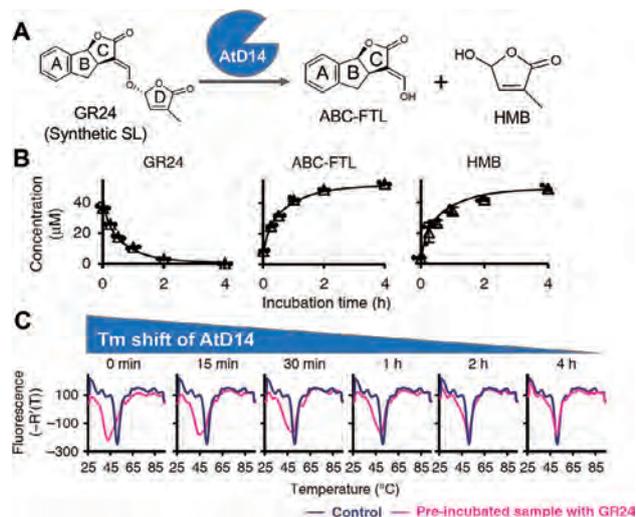


Figure 1. The time-course analyses of SL binding and hydrolysis by AtD14. (A) Hydrolysis reaction of SL (GR24) by AtD14. (B) Quantification of the hydrolysis reaction of GR24 (40 μ M) by AtD14. (C) The T_m shift of AtD14 incubated with GR24 (40 μ M) in DSF analysis. The maximum T_m shift was observed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

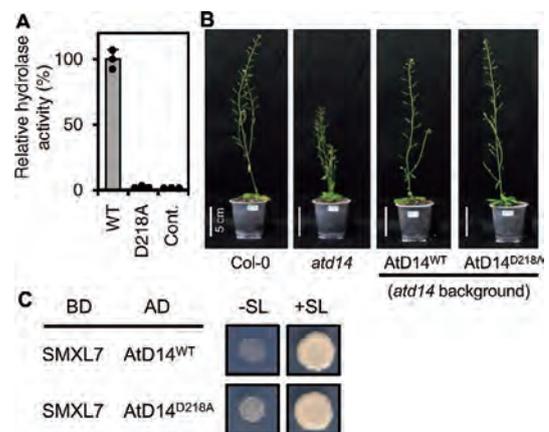


Figure 2. Functional analysis of the AtD14^{D218A} mutant. (A) The SL hydrolysis activities of maltose binding protein (MBP)-tagged wild-type of AtD14 protein (AtD14^{WT}) and the AtD14^{D218A} mutant. MBP was used in the control reaction. (B) The branching phenotype of Arabidopsis transgenic plants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

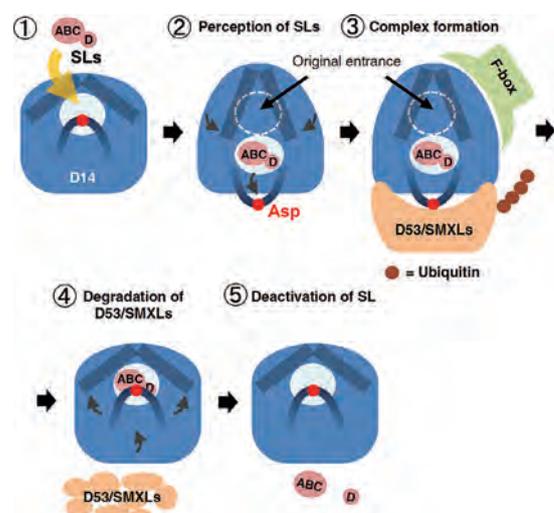


Figure 3. A proposed model of D14 in SL signaling. Bioactive SLs induce the conformational changes of D14, which triggers complex formation with the signaling partners. After the degradation of negative regulators of SL signaling (D53/SMXLs) and transmission of the SL signal, D14 reconstructs the catalytic 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
Phospholipid Signaling
RNA
Signal Transduction
COP9 Signalosome



Recent Selected Publications

Shimamura, R.; Ohashi, Y.; Taniguchi, Y.Y.; Kato, M.; Tsuge, T.; Aoyama, T., Arabidopsis PLD ζ 1 and PLD ζ 2 Localize to post-Golgi Membrane Compartments in a Partially Overlapping Manner, *Plant Mol. Biol.*, DOI: 10.1007/s11103-021-01205-0 (2021).
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Aki, S.S.; Yura, K.; Aoyama, T.; Tsuge, T., SAPI30 and CSN1 Interact and Regulate Male Gametogenesis in *Arabidopsis thaliana*, *J. Plant Res.*, **134**, 279-289 (2021).
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Cleavage Factor I Regulates the Diversity of 3' UTR ends in mRNA Processing

In eukaryotes, gene expression is exercised by the transcription of DNA into mRNA in the nucleus. During this process, mRNA precursor (pre-mRNAs) undergoes a series of processing events, including its' cleavage at the 3' end that then leads to addition of a polyadenosine tail. Cleavage and polyadenylation at the 3' end of the pre-mRNA not only plays an important role in the transport and stability of the transcript but also in the transcription and the translation events. Once pre-mRNAs are processed to mature, they are subjected to protein synthesis and other regulatory functions in the cytoplasm.

Cleavage Factor I (CFI) is a nuclear protein complex that functions in the pre-mRNA 3' end processing machinery that determines the polyadenylation site, among potential selections. Mammalian CFI is a tetramer composed of two CFI 25s and another two subunits of either CFI 59 and/or CFI 68. In *Arabidopsis thaliana*, a model plant for dicots, AtCFI 25a, AtCFI 25b, AtCFI 59, AtCFI 68 were identified as orthologs. The loss of function of *AtCFI 25a*, but not *AtCFI 25b*, showed pleiotropic developmental defects such as, small rosette leaf, reduced lamina pigmentation, undeveloped stamen with less pollen grains, abnormally elongated papillary cells, short primary root, and less secondary roots, when compared to wild type (Figure 1). Furthermore, the length of the silique and fertility was severely reduced in *atcfi 25a* (Figure 2). Hence, *AtCFI 25a* function was essential for proper development of plant architecture.

3' RACE analyses on mRNAs of *AtCFI 25b*, *AtCFI 59*, and *AtCFI 68* revealed that *AtCFI 25a* function was essential to maintain the diverse pattern of 3' UTR length, observed in the wild-type plants (Figure 3). This suggested a self-regulating mechanism of the plant CFI. Preliminary results indicate that this function of *AtCFI 25a* in 3' end processing of pre-mRNA, seemed to affect a number of genes that are involved in various processes of development to different extents. It is interesting to note that the loss of CFI function in plants not only leads to proximal selection of the given transcript, as had been proposed in mammals, but fails to maintain the diversity of 3' UTR end selection. This is a novel finding *via* taking advantage of the plant model system. Although further investigation is in progress, we hypothesize that gene expression is modulated through the selection of diverse cleavage and polyadenylation sites on the given transcript, which in turn, not only adds diversity to the limited DNA template resource, but also facilitates multiple level of regulation in development and environmental responses.

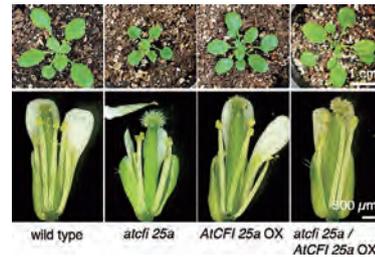


Figure 1. *AtCFI 25a* function is essential for plant morphogenesis. Null *atcfi 25a*, loss of function plants of *AtCFI 25a*, display pleiotropic defects, such as smaller aerial structure (upper panels) and deformed flower organs (lower panels). Overexpression of *AtCFI 25a* in wild-type background causes no obvious phenotypic difference when compared to wild type, however it partially complements the abnormality observed in *atcfi 25a*, when expressed in *atcfi 25a* background. Some petals and sepals were removed to show the flower structure. Lengths of scale bars are noted in the figure.

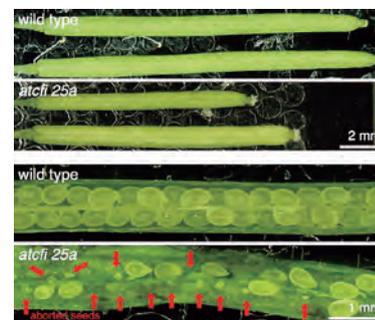


Figure 2. *atcfi 25a* displays low fertility due to abnormal flower organ development. Morphological comparison of wild type and *atcfi 25a* show that *AtCFI 25a* function is essential for maintaining proper length of the silique (upper panels) and seed formation (lower panels). Red arrows show the aborted seeds leading to low fertility. Lengths of scale bars are noted in the figure.

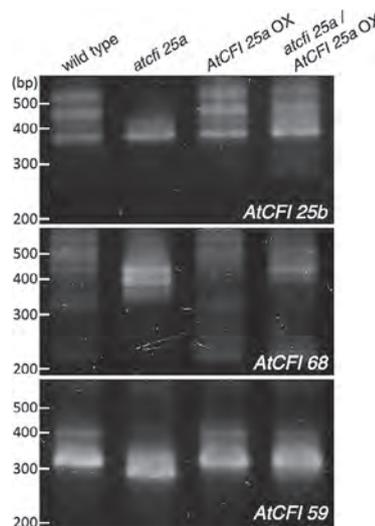


Figure 3. Comparison of cleavage and polyadenylation sites of wild type, *atcfi 25a*, *AtCFI 25a OX*, and *atcfi 25a-3 / AtCFI25a OX* for genes encoding putative CFI subunits. 3' RACE amplifications of *AtCFI 25a*, *AtCFI 25b*, *AtCFI 68*, and *AtCFI 59* are shown as comparable gel patterns on agarose gel after electrophoresis. Note that the of the 3' UTR length pattern is less diverse in *atcfi 25a* while those in *AtCFI 25a OX* and *atcfi 25a-3 / AtCFI25a OX* is similar to wild type. Bands were confirmed to represent 3' UTR of each gene through sequencing. Subjected samples: 7 DAS seedlings.

Division of Biochemistry

– Chemical Biology –

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Scope of Research

Chemical biology is an interdisciplinary field of study that is often defined as “chemistry-initiated biology.” As biological processes all stem from chemical events, it should be possible to understand or manipulate biological events using chemistry. Our laboratory has been discovering or designing unique organic molecules that modulate fundamental processes in human cells. Such synthetic organic molecules often serve as tools for basic cell biology. Discovery or design of small molecules with unique biological activities permits small-molecule-initiated exploration of complex cellular events. Our mission is to create a new world of bioactive synthetic molecules: new modes of activity, new shapes, and new sizes. We hope that these basic studies open new avenues for small-molecule applications in a range of fields.

KEYWORDS

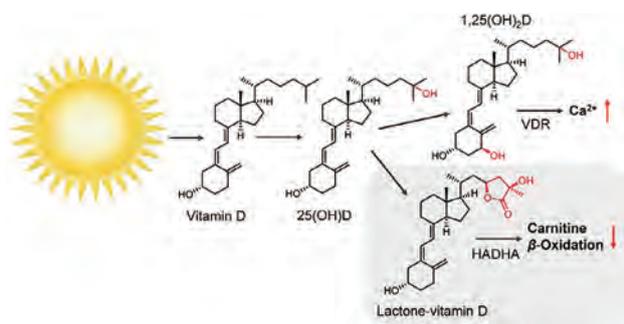
Chemical Biology Small Molecules Chemical Library
Chemical Genetics Immunology

Recent Selected Publications

Mendoza, A.; Takemoto, Y.; Cruzado, K. T.; Masoud, S. S.; Nagata, A.; Tantipanjaporn, A.; Okuda, S.; Kawagoe, F.; Sakamoto, R.; Odagi, M.; Mototani, S.; Togashi, M.; Kawatani, M.; Aono, H.; Osada, H.; Nakagawa, H.; Higashi, T.; Kittaka, A.; Nagasawa, K.; Uesugi, M., Controlled Lipid β -Oxidation and Carnitine Biosynthesis by a Vitamin D Metabolite, *Cell Chem Biol.*, (2021) (in press).
Takemoto, Y.; Kadota, S.; Minami, I.; Otsuka, S.; Okuda, S.; Abo, M.; Punzalan, L. L.; Shen, Y.; Shiba, Y.; Uesugi, M., Chemical Genetics Reveals a Role of Squalene Synthase in TGF β Signaling and Cardiomyogenesis, *Angew. Chem. Int. Ed.*, **60**, 21824-21831 (2021).
Jin, S.; Vu, H. T.; 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**, 961-969 (2021).
Hakariya, H.; Takashima, I.; Takemoto, M.; Noda, N.; Sato, S.; Uesugi, M., Non-Genetic Cell-Surface Modification with a Self-Assembling Molecular Glue, *Chem. Commun.*, **57**, 1470-1473 (2021).
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).

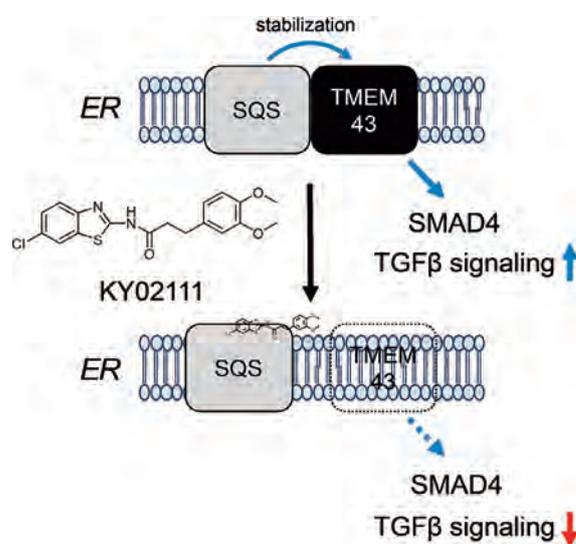
Controlled Lipid β -Oxidation and Carnitine Biosynthesis by a Vitamin D Metabolite

Lactone-vitamin D3 is a major metabolite of vitamin D3, a lipophilic vitamin biosynthesized in numerous life forms by sunlight exposure. Although lactone-vitamin D3 was discovered 40 years ago, its biological role remains largely unknown. Chemical biological analysis of its photoaffinity probe identified the hydroxyacyl-CoA dehydrogenase trifunctional multienzyme complex subunit alpha (HADHA), a mitochondrial enzyme that catalyzes β -oxidation of long-chain fatty acids, as its selective binding protein. Intriguingly, the interaction of lactone-vitamin D3 with HADHA does not affect the HADHA enzymatic activity but instead limits biosynthesis of carnitine, an endogenous metabolite required for the transport of fatty acids into the mitochondria for β -oxidation. Lactone-vitamin D3 dissociates the protein-protein interaction of HADHA with trimethyllysine dioxygenase (TMLD), thereby impairing the TMLD enzyme activity essential in carnitine biosynthesis. These findings suggest a heretofore undescribed role of lactone-vitamin D3 in lipid β -oxidation and carnitine biosynthesis, and possibly in sunlight-dependent shifts of lipid metabolism in animals.



Chemical Genetics Reveals a Role of Squalene Synthase in TGF β Signaling and Cardiomyogenesis

KY02111 is a widely used small molecule that boosts cardiomyogenesis of the mesoderm cells derived from pluripotent stem cells, yet its molecular mechanism of action remains elusive. The present study resolves the initially perplexing effects of KY02111 on Wnt signaling and subsequently identifies squalene synthase (SQS) as a molecular target of KY02111 and its optimized version, KY-I. By disrupting the interaction of SQS with cardiac ER-membrane protein TMEM43, KY02111 impairs TGF β signaling, but not Wnt signaling, and thereby recapitulates the clinical mutation of TMEM43 that causes arrhythmogenic right ventricular cardiomyopathy (ARVC), an inherited heart disease that involves a substitution of myocardium with fatty tissue. These findings reveal a heretofore undescribed role of SQS in TGF β signaling and cardiomyogenesis. KY02111 may find its use in ARVC modeling as well as serve as a chemical tool for studying TGF β /SMAD signaling.



Division of Environmental Chemistry – Molecular Materials Chemistry –

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Scope of Research

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

KEYWORDS

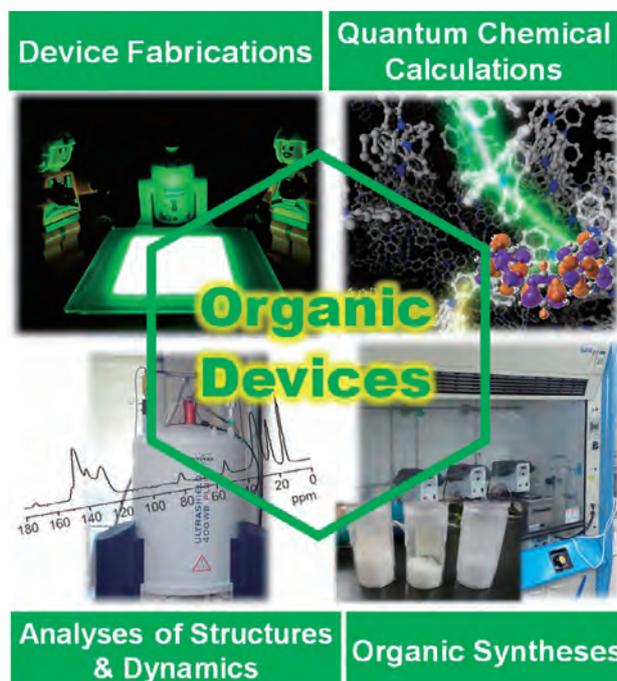
Organic Light-Emitting Diodes

Solid-State NMR

Quantum Chemical Calculation

Amorphous Materials

Dynamic Nuclear Polarization Enhanced NMR



Recent Selected Publications

Shizu, K.; Kaji, H., Theoretical Determination of Rate Constants from Excited-States: Application to Benzophenone, *J. Phys. Chem. A*, **125**, 9000-9010 (2021).

Ren, Y.; Wada, Y.; Suzuki, K.; Kusakabe, Y.; Geldsetzer, J.; Kaji, H., Efficient Blue Thermally Activated Delayed Fluorescence Emitters Showing Very Fast Reverse Intersystem Crossing, *Appl. Phys. Express*, **14**, [071003-1]-[071003-5] (2021).

Wada, Y.; Shizu, K.; Kaji, H., Molecular Vibration Accelerates Charge Transfer Emission in a Highly Twisted Blue Thermally Activated Delayed Fluorescence Material, *J. Phys. Chem. A*, **125**, 4534-4539 (2021).

Theoretical Determination of Rate Constants for Materials Screening

Theoretical prediction of rate constants has attracted great attention because of its relevance to materials chemistry. We report a cost-effective method of theoretically predicting electronic transition rate constants from the excited states of molecules. Our method is based on quantum chemical calculations of electronic states and the Fermi golden rule. We apply the method to the excited-state decay mechanism of photoexcited benzophenone and show that calculated rate constants, including radiative (fluorescence) and nonradiative decays from S_1 to S_0 , radiative decay (phosphorescence) from T_1 to S_0 , and intersystem crossing from S_1 to T_2 , are quantitatively in good agreement with the experimental ones. From the calculated population kinetics, a stepwise $S_1 \rightarrow T_2 \rightarrow T_1 \rightarrow S_0$ transition is found to be the predominant decay pathway. The direct $S_1 \rightarrow T_1$ transition is suppressed owing to a fast $S_1 \rightarrow T_2$ intersystem crossing. Our method of predicting rate constants is useful for accelerating materials screening.

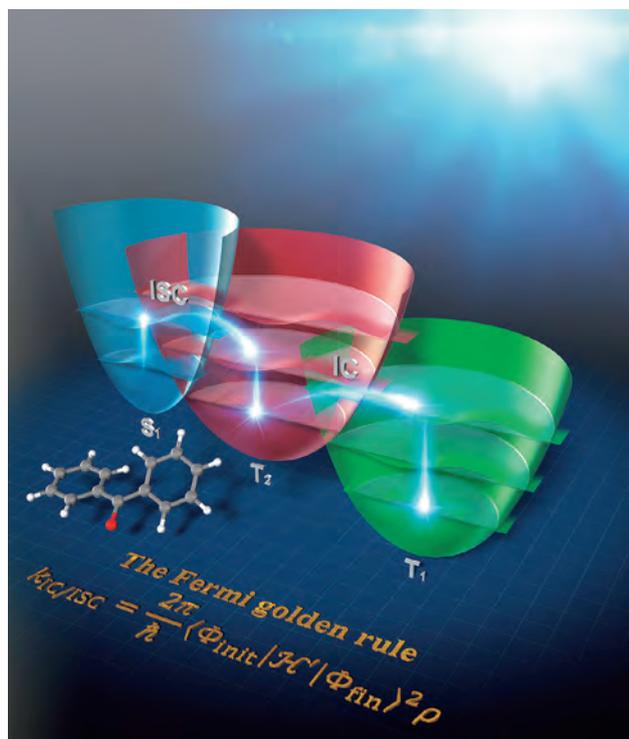


Figure 1. A stepwise $S_1 \rightarrow T_2 \rightarrow T_1$ decay mechanism of photoexcited benzophenone.

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.

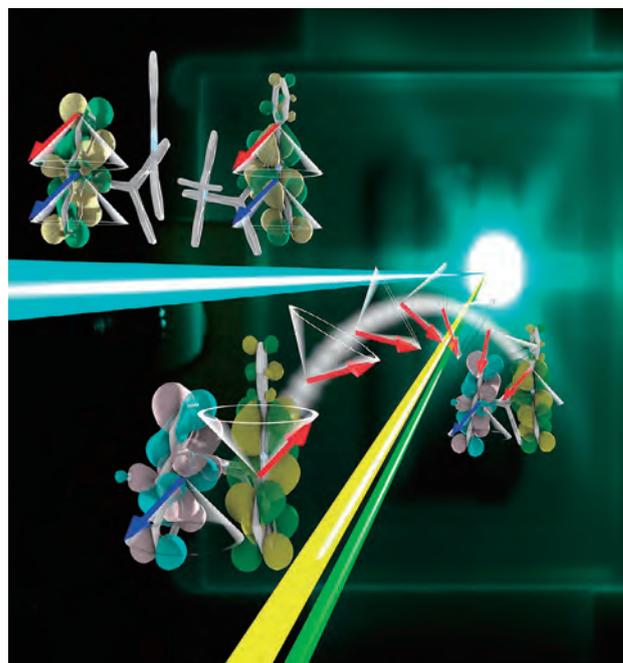


Figure 2. A thermally activated delayed fluorescence molecule showing very fast reverse intersystem crossing.

Division of Environmental Chemistry

– Hydrospheric Environment Analytical Chemistry –

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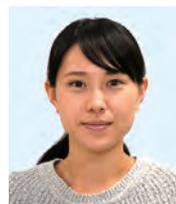
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MATSUOKA, Kohei (M1)

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

Recent Selected Publications

Liao, W.-H.; Takano, S.; Tian, H.-A.; Chen, H.-Y.; Sohrin, Y.; Ho, T.-Y., Zn Elemental and Isotopic Features in Sinking Particles of the South China Sea: Implications for Its Sources and Sinks, *Geochim. Cosmochim. Acta.*, **314**, 68-84 (2021).

Sakata, K.; Takahashi, Y.; Takano, S.; Matsuki, A.; Sakaguchi, A.; Tanimoto, H., First X-ray Spectroscopic Observations of Atmospheric Titanium Species: Size Dependence and the Emission Source, *Environ. Sci. Technol.*, **55**, 10975-10986 (2021).

Zheng, L.; Minami, T.; Takano, S.; Ho, T.-Y.; Sohrin, Y., Sectional Distribution Patterns of Cd, Ni, Zn, and Cu in the North Pacific Ocean: Relationships to Nutrients and Importance of Scavenging, *Glob. biogeochem. Cycles.*, **35**, e2020GB006558 (2021).

Takano, S.; Tsuchiya, M.; Imai, S.; Yamamoto, Y.; Fukami, Y.; Suzuki, K.; Sohrin, Y., Isotopic Analysis of Nickel, Copper, and Zinc in Various Freshwater Samples for Source Identification, *Geochim. J.*, **55(3)**, 171-183 (2021).

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*, **77**, 463-485 (2021).

Sectional Distribution Patterns of Cd, Ni, Zn, and Cu in the North Pacific Ocean: Relationships to Nutrients and Importance of Scavenging

The North Pacific Ocean is located at the end of the thermohaline circulation of deep water. This study reports on basin-scale full-depth sectional distributions of total dissolvable (td), dissolved (d), and labile particulate (lp) Cd, Ni, Zn, and Cu along three transects: the GEOTRACES transects GP18 (165°E) and GP02 (47°N), and along 160°W. We find that scavenging is an important factor that significantly affects the distributions of dZn, dNi, and dCu, of which the magnitude of influence increases in the order of Cd < Ni, Zn < Cu. The relationships between the four dissolved metals with Si(OH)₄ and PO₄ differed considerably from those in other oceans. The spot concentration ratio of dCd/PO₄ was 0.34 ± 0.02 nmol/μmol ($n = 296$) in waters >800 m deep, which is in the range of the phytoplankton Cd/P ratio. This is indicative of the dominant effect of water circulation and biological processes on dCd distribution. The dissolved metals (dMs) to PO₄ ratios of other examined metals were either partially or completely outside the range of typical biomass ratios. They generally increased with depth in waters >800 m deep; the magnitude of increase was the highest for Cu and moderate for Ni and Zn. Below 800 m, an increase in the apparent oxygen utilization from 150 to 300 μmol/kg was concurrent with a decrease in the dMs/PO₄ ratios: $4 \pm 3\%$ for Cd, $21 \pm 4\%$ for Zn, $21 \pm 3\%$ for Ni, and $69 \pm 7\%$ for Cu.

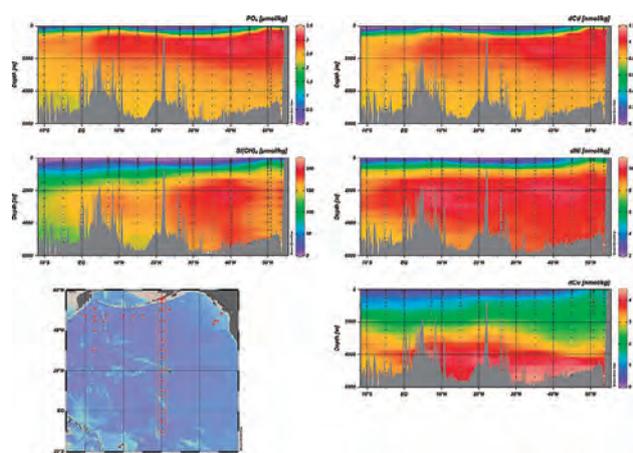


Figure 1. Full-depth sectional distributions of PO₄, Si(OH)₄, dCd, dNi, and dCu along 160°W.

Constraints on Redox Conditions in the Japan Sea in the Last 47,000 Years Based on Mo and W as Palaeoceanographic Proxies

Both molybdenum (Mo) and tungsten (W) form soluble oxyanions in oxic seawater, whereas Mo forms insoluble thiomolybdate and W forms soluble thiotungstate in sulfidic seawater. Thus, concentrations and stable isotope ratios of Mo and W in sediments may fluctuate due to changes in redox conditions and can be used to estimate paleoenvironmental changes. The modern Japan Sea is oxic from the surface to the bottom, whereas deep water became anoxic several times from the late Pleistocene to the Holocene. Detailed information on redox conditions is still lacking. In this study, we analyzed a sediment core that was collected from offshore Iwanai, Hokkaido (43°22'36" N, 140°04'10" E, water depth 900 m). To the best of our knowledge, our study is the first to report stable isotope data of Mo and W in sediments of the Japan Sea. We observed maxima in the Mo concentration of up to 29 ppm in the sediment layers of 11–10 ka, 17–14 ka (the last glacial maximum), 31 ka, and 45 ka in accordance with the maxima of total sulfur, thereby indicating the deposition of thiomolybdate MoO₃S_{4-x}²⁻ ($0 \leq x \leq 3$). δ⁹⁸Mo, however, was between -0.19 and 0.69‰ at these ages, suggesting that the H₂S concentration in bottom water never exceeded 11 μmol kg⁻¹. The concentration and isotopic ratio of W were relatively constant throughout the core; W = 1.2 ± 0.2 ppm and δ¹⁸⁶W = $0.03 \pm 0.03\%$ (ave ± sd). The authigenic Mo and W ratio, Mo_{auth}/W_{auth} (mol/mol), was 10.5 ± 7.3 except for the above four ages, supporting the control of Mn and Fe(oxyhydr)oxides on Mo_{auth} and W_{auth} under oxic conditions.

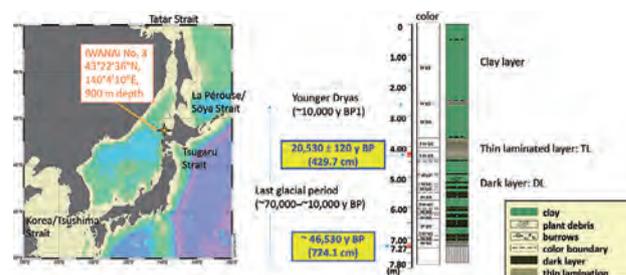


Figure 2. Sampling site and appearance of the sediment core.

Division of Environmental Chemistry – Chemistry for Functionalized Surfaces –

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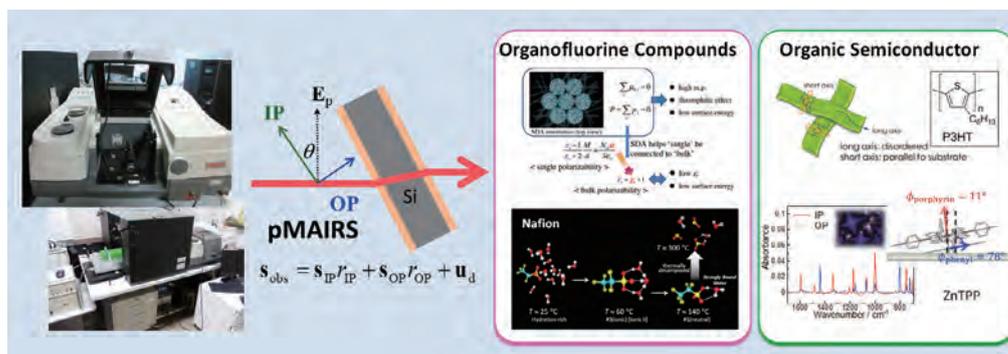
FANG, Tao (M1)

Scope of Research

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

KEYWORDS

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



Recent Selected Publications

Tomita, K.; Shioya, N.; Shimoaka, T.; Okudaira, K. K.; Yoshida, H.; Koganezawa, T.; Hasegawa, T., Substrate-Independent Control of Polymorphs in Tetraphenylporphyrin Thin Films by Varying the Solvent Evaporation Time Using a Simple Spin-Coating Technique, *Cryst. Growth Des.*, **21**, 5116-5125 (2021).

Shioya, N.; Fujiwara, R.; Tomita, K.; Shimoaka, T.; Okudaira, K. K.; Yoshida, H.; Koganezawa, T.; Hasegawa, T., Monitoring of Crystallization Process in Solution-Processed Pentacene Thin Films by Chemical Conversion Reactions, *J. Phys. Chem. C*, **125**, 2437-2445 (2021).

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

Shimoaka, T.; Sonoyama, M.; Amii, H.; Takagi, T.; Kanamori, T.; Hasegawa, T., Raman Optical Activity on a Solid Sample: Identification of Atropisomers of Perfluoroalkyl Chains Having a Helical Conformation and No Chiral Center, *J. Phys. Chem. A*, **123**, 3985-3991 (2019).

Hasegawa, T., Physicochemical Nature of Perfluoroalkyl Compounds Induced by Fluorine, *Chem. Rec.*, **17**, 903-917 (2017).

Substrate-independent Control of Polymorphs in Tetraphenylporphyrin Thin Films by Varying the Solvent Evaporation Time Using a Simple Spin-coating Technique

Porphyrin derivatives are promising materials for various thin-film-based devices such as solar cells, field-effect transistors, and gas sensors. Since the molecular aggregation structure in a thin film significantly influences the device performance, controlling the aggregation structure is of crucial importance. In this study, we show that three different crystalline polymorphs of free-base tetraphenylporphyrin can be made to form in spin-coated thin films depending on the evaporation time of the solvent. The crystal structure in the films is identified using a combination of the two-dimensional grazing incidence X-ray diffraction (2D-GIXD) and p-polarized multiple-angle incidence resolution spectroscopy (pMAIRS) techniques. The results show that the aggregation structure in the as-spun films is controlled by the solvent evaporation time, and the initial film structure determines the polymorphs obtained after thermal annealing.

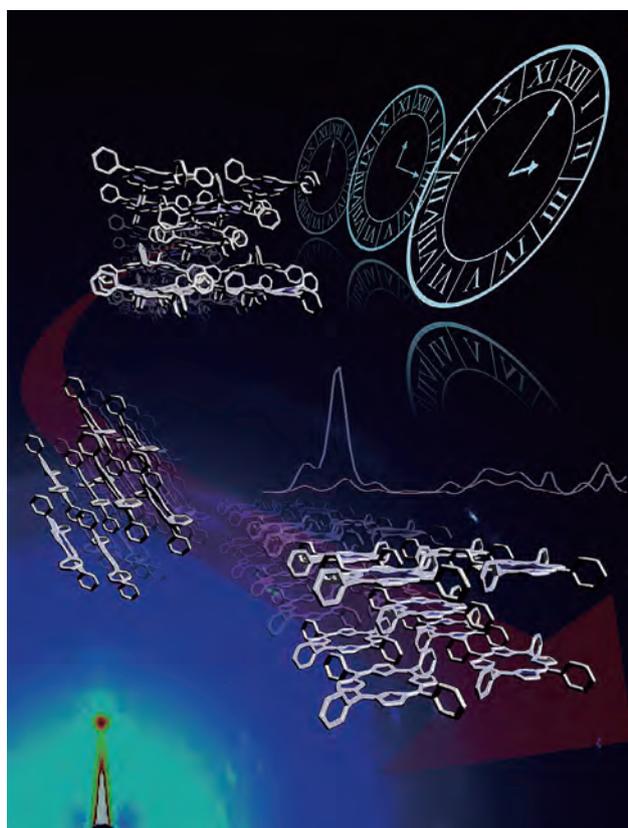


Figure 1. Three different tetraphenylporphyrin crystal structures are selectively obtained on an inert surface by varying the evaporation time of the solvent.

Monitoring of Crystallization Process in Solution-processed Pentacene Thin Films by Chemical Conversion Reactions

Solution-processable organic semiconductors having bulky substituent groups on the π -conjugated skeleton are rapidly gaining attention for their potential applications to large-area electronics. While the substituent groups contribute to the good solubility in organic solvents, they give rise to hopping sites in a thin film, affecting adversely the charge-carrier transport. As an alternative material, a solvent-soluble precursor compound with thermally cleavable functional groups is promising, which can be converted by heat treatment into a thin film to generate the desired material consisting solely of conjugated systems. This precursor approach is practically applied to various thin-film-based devices. The overall process of the thin film growth, however, remains unrevealed. In the present study, solution-processed pentacene thin films are prepared from a thermally convertible precursor, and the structural evolution during the chemical conversion reaction has been revealed by employing multiple analytical techniques of 2D-GIXD, pMAIRS, and atomic force microscopy. The highlight is that pentacene is crystallized in a stepwise manner in the thermally converted films, which is substantially different from a typical growth process. In addition, influences of the oxidation reaction of pentacene on the molecular arrangement are also discussed using the pMAIRS technique. The spectra quantitatively reveal that the presence of oxidation products disturbs molecular orientation of pentacene. This study provides a fundamental schematic of thin films grown by the precursor method.

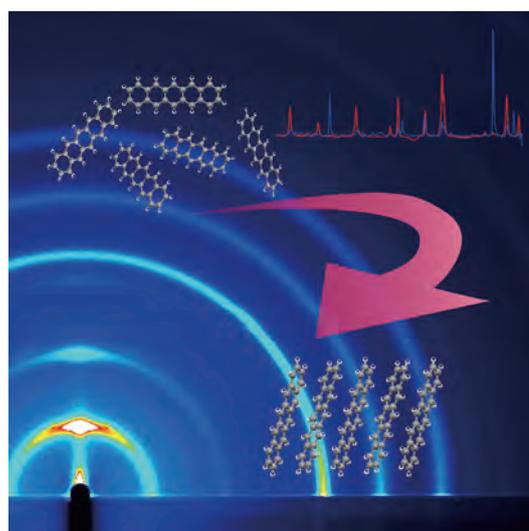


Figure 2. A combination of 2D-GIXD and pMAIRS reveal a complex growth process of solution-processed pentacene thin films, including the structural conversion reaction.

Division of Environmental Chemistry – Molecular Microbial Science –

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MASAKI, Asuka (M1)

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

Bacterial Cold-adaptation Mechanism

Polyunsaturated Fatty Acid

Phospholipid Acyltransferase

Extracellular Membrane Vesicle

Recent Selected Publications

- Yokoyama, F.; Imai, T.; Aoki, W.; Ueda, M.; Kawamoto, J.; Kurihara, T., Identification of a Putative Sensor Protein Involved in Regulation of Vesicle Production by a Hypervesiculating Bacterium, *Shewanella vesiculosa* HM13, *Frontiers in Microbiology*, **12**, 629023 (2021).
- 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, *Frontiers in Microbiology*, **10**, 3001 (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).
- Ogawa, T.; Hirose, K.; Yusuf, Y.; Kawamoto, J.; Kurihara, T., Bioconversion from Docosahexaenoic Acid to Eicosapentaenoic Acid in the Marine Bacterium *Shewanella livingstonensis* Ac10, *Frontiers in Microbiology*, **11**, 1104 (2020).

Study on the Roles of Multiple Lysophosphatidic Acid Acyltransferases in Bacteria

Phospholipids (PLs), which are major constituents of biological membranes, comprise fatty acyl groups that vary in their chemical structures (*e.g.*, carbon chain length and unsaturation level) and correspondingly form PL membranes with various physical properties (*e.g.*, fluidity and thickness). Bacteria control the fatty acid compositions of the PL membranes in response to environmental changes to maintain membrane integrity. Lysophosphatidic acid acyltransferase (LPAAT), which is an enzyme that introduces an *sn*-2 fatty acid of PLs during their biosynthesis, is a regulator for the membrane fatty acid compositions. Many bacteria have multiple LPAAT paralogs, suggesting that these enzymes differ in functions, localizations, and timing of expression, and their coordinated actions enable the accurate regulation of membrane fatty acid compositions. We have been studying the LPAAT multiplicity using the marine bacterium *Shewanella livingstonensis* Ac10, which has five LPAATs (designated as PlsC1–PlsC5). To understand their division of roles, we studied the enzymatic and physiological functions of the two closely homologous LPAATs, PlsC4 and PlsC5. Mutagenesis analysis revealed that PlsC4 selectively utilizes *iso*-tridecanoic acid (medium-chain length and methyl-branched) for PL production, while PlsC5 prefers hexadecenoic acid (long-chain length and monounsaturated), thus generating PLs with different physicochemical properties. Consistent with a beneficial effect of branched-chain fatty acids in bacterial cold-adaptation, the *plsC4*-deficient cell grew slower than the *plsC5*-deficient and parent cells at 4 °C, whereas their growth was comparable at 18 °C. In addition, bioinformatic analysis indicated that the two LPAAT paralogs, which are distant from principal LPAATs, are widely distributed among γ -proteobacteria such as *Escherichia*, *Pseudomonas*, and *Vibrio*. Therefore, regulation of the membrane fatty acid compositions by multiple LPAATs might be more common than previously considered.

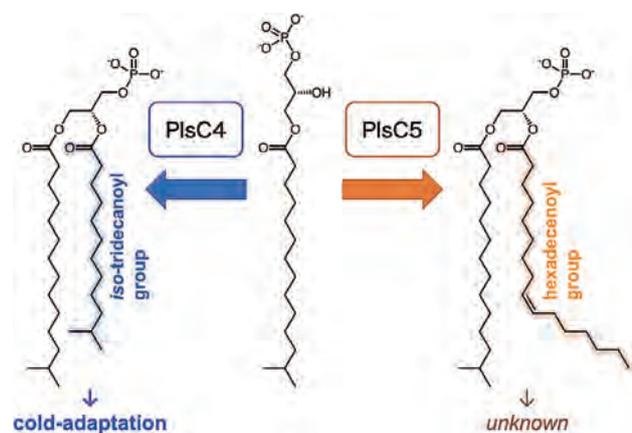


Figure 1. PlsC4 and PlsC5 are selective to different fatty acyl donor substrates and produce distinct PLs.

Construction of a Hypervesiculation Strain of *Shewanella vesiculosa* HM13 to Develop a Secretory Protein Production System at Low Temperatures

Bacteria secrete spherical nanoparticles enclosed by lipid membranes called extracellular membrane vesicles (EMVs), which selectively transport various biomolecules, including nucleic acids, lipids, lipopolysaccharides, and proteins, to their extracellular environments. EMVs serve a number of important roles in microbial interactions and survival in hostile environments. Besides, EMVs have attracted the attention of biotechnological industries for their potential use as a platform of vaccine, drug-delivery systems, and recombinant protein production systems.

Shewanella vesiculosa HM13, a psychrotrophic Gram-negative bacterium isolated from the intestinal contents of horse mackerel, abundantly produces EMVs carrying a single major cargo protein, P49, of unknown function and thus has a great potential for the secretory production of heterologous proteins. In Gram-negative bacteria, the outer membrane is connected to the peptidoglycan predominantly through Braun's lipoprotein (Lpp), and the formation of this linkage is catalyzed by L,D-transpeptidase (Ldt). The importance of this linkage for cell membrane stability implies that its disruption may lead to increased EMV production. In this study, to enhance the EMV productivity of *S. vesiculosa* HM13, we identified and disrupted genes coding for proteins involved in the outer membrane integrity, Lpp and Ldt. According to the bioinformatics analysis using amino acid sequences of *E. coli* Lpp and Ldt, we found genes coding for these protein homologs in the genome of *S. vesiculosa* HM13. These proteins have sequence similarities of 34.8% and 59.8% to those of *E. coli*, respectively. *lpp*- and *ldt*-gene disrupted mutants, Δ Lpp and Δ Ldt, generated by single crossover recombination demonstrated normal growth characteristics compared to the wild type. Next, we analyzed their EMV productivity, size distribution, and morphology. As a result, about 2.5-fold increase in EMV production was observed for Δ Lpp and Δ Ldt, while the morphology of EMVs of these mutants remained identical to those of the parent strain. In accordance with the increase in EMV production, the mutants secreted 2.3–2.5 mg/OD₆₀₀·L of P49 into the culture broth through EMVs as the cargo (Figure 2), which is around two times of the parent strain. These findings will contribute to the development of the EMV-based protein production system by using *S. vesiculosa* HM13 as the host.

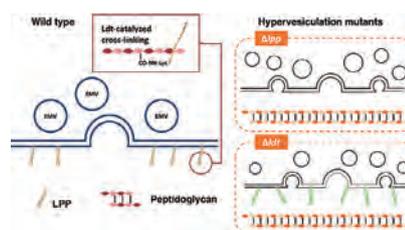


Figure 2. Schematic model of hypervesiculation strain of *Shewanella vesiculosa* HM13.

Division of Multidisciplinary Chemistry – Polymer Materials Science –

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



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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



Recent Selected Publications

Takenaka, M.; Nishitsuji, S.; Watanabe, Y.; Yamaguchi, D.; Koizumi, S., Analyses of Hierarchical Structures in Vulcanized SBR Rubber by Using Contrast-Variation USANS and SANS, *J. Appl. Cryst.*, **54**, 949-956 (2021).

Nakanishi, Y.; Mita, K.; Yamamoto, K.; Ichino, K.; Takenaka, M., Effects of Mixing Process on Spatial Distribution and Coexistence of Sulfur and Zinc in Vulcanized EPDM Rubber, *Polymer*, **218**, 123486 (2021).

Ogawa, H.; Takenaka, M.; Miyazaki, T., Molecular Weight Effect on the Transition Processes of a Symmetric PS-b-P2VP during Spin-Coating, *Macromolecules*, **54**, 1017-1029 (2021).

Effects of Mixing Process on Spatial Distribution and Coexistence of Sulfur and Zinc in Vulcanized EPDM Rubber

The vulcanization of rubbers is attained by the mechanical mixing of rubbers, sulfur and zinc oxide (ZnO). Sulfur crosslinks the rubber by reacting to double bonds in the rubber and ZnO accelerates the vulcanization of the rubbers with sulfur efficiently. The amount of coexistence of sulfur and ZnO is an important factor to attain the effective crosslink as well as their dispersion. We have successfully observed spatial distributions of sulfur and zinc and their spatial correlation in vulcanized ethylene-propylene-diene copolymer (EPDM) rubber by using Microscopic X-ray fluorescence mapping with synchrotron radiation. We found the mixing processes strongly affected the amount of coexistence of sulfur and ZnO as well as the spatial distributions of each component. The better spatial cross-correlation and homogeneity of sulfur and zinc improved the performance of the EPDM rubber.

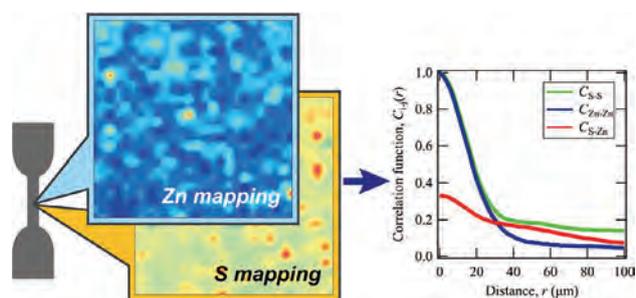


Figure 1. The μ -XRF mapping images of the vulcanized EPDM samples.

Artifact Removal in the Contour Areas of SAXS-CT Images by Tikhonov-L1 Minimization

Small-angle X-ray scattering (SAXS) coupled with computed tomography (CT), denoted SAXS-CT, has enabled the spatial distribution of the characteristic parameters (*e.g.*, size, shape, surface, characteristic length) of the nanoscale structures inside samples to be visualized. In this experimental geometry, we often face to the serious problem that the reflection of incident X-rays interferes with the 2D SAXS patterns near the sample edge which kinds of anomalous scattering (artifact) seriously damage the reconstructed CT image. We attempted to remove streak-derived intensities as noise from the sinogram by implementing Tikhonov-L1 optimization. We treated the removal procedure of the streak-derived noise as a constrained convex optimization problem, where we imposed Tikhonov-type regularization on the sinogram to exploit the underlying smoothness of the sinogram and used L1 norm regularization to characterize the sparsity of streak-derived noise. For a sample, we employed a crystalline polymer exhibiting an isotropic peak in the SAXS scattering pattern originating from lamellar structures. We successfully removed the noise due to streak scattering from the sinogram image and were able to reconstruct the CT image free from artifacts in the contour regions. This technique is useful for removing spot-like noise not only for SAXS-CT but also for conventional X-ray CT.

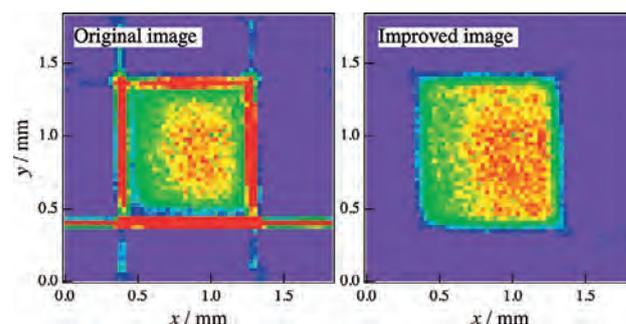


Figure 2. Original and improved CT images from the sinogram of the signal components.

Division of Multidisciplinary Chemistry

– Molecular Rheology –

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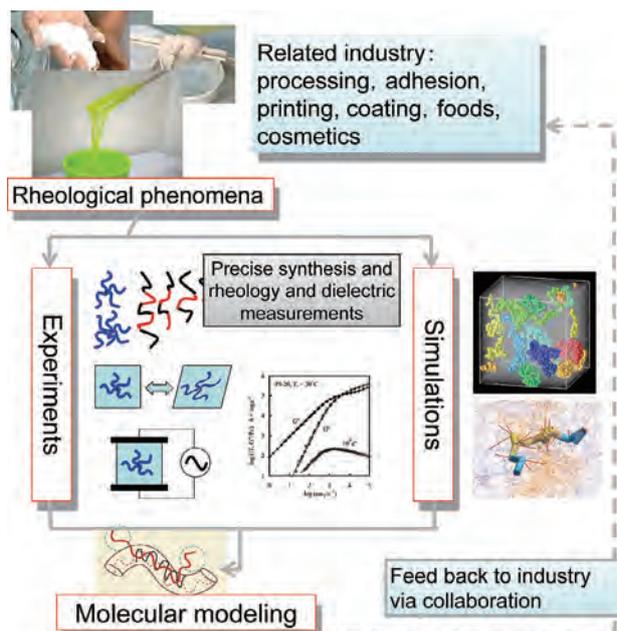
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Scope of Research

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



Recent Selected Publications

Sato, T.; Kwon, Y.; Matsumiya, Y.; Watanabe, H., A Constitutive Equation for Rouse Model Modified for Variations of Spring Stiffness, Bead Friction, and Brownian Force Intensity Under Flow, *Phys. Fluids*, **33**, 063106 (2021).

Matsumiya, Y.; Watanabe, H.; Sukhonthamethirat, N.; Vao-Soongnern, V., Viscoelastic and Dielectric Behavior of Polyisoprene Monofunctionally Head-Modified with Associative Metal-Carboxylate Group, *J. Soc. Rheol. Jpn.*, **49**, 189-197 (2021).

Shimada, R.; Urakawa, O.; Inoue, T.; Watanabe, H., Phase Equilibrium and Dielectric Relaxation in Mixture of 5CB with Dilute Dimethyl Phthalate: Effect of Coupling between Orientation and Composition Fluctuations on Molecular Dynamics in Isotropic One-Phase State, *Soft Matter*, **17**, 6259-6272 (2021).

Watanabe, H.; Matsumiya, Y.; Sato, T., Revisiting Nonlinear Flow Behavior of Rouse Chain: Roles of FENE, Friction-Reduction, and Brownian Force Intensity Variation, *Macromolecules*, **54**, 3700-3715 (2021).

Matsumiya, Y.; Watanabe, H., Non-Universal Features in Uniaxially Extensional Rheology of Linear Polymer Melts and Concentrated Solutions: A Review, *Prog. Polym. Sci.*, **112**, 101325 (2021).

Revisiting Nonlinear Flow Behavior of Rouse Chain: Roles of FENE, Friction-Reduction, and Brownian Force Intensity Variation

The local elastic strength κ , segmental friction coefficient ζ , and the Brownian force intensity B of polymer chains in a melt are expected to change under fast flow. This study examined the effects of those changes on rheological and structural properties of the Rouse model, the most frequently utilized model for unentangled melts. Specifically, the Langevin equation of the Rouse model was solved with the decoupling and preaveraging approximations to derive analytical expressions of nonlinear rheological properties and the end-to-end stretch ratio under steady shear and extension. The expressions explicitly included nonequilibrium parameters r_κ , r_ζ , and r_B defined as the ratios of κ , ζ , and B under flow to those at equilibrium, thereby offering a method of evaluating each of r_κ , r_ζ , and r_B from rheological and structural data under flow within the framework of those approximations. Data of extensional viscosity η_E and the relaxation rate of the tensile stress decay coefficient η_E^- reported for the unentangled polystyrene melt (PS-27k; $M = 27.1 \times 10^3$) and data of shear viscosity η and the first normal stress difference coefficient Ψ_1 reported for the PS-14k melt ($M = 13.7 \times 10^3$) were analyzed with this method to evaluate the r_ζ/r_κ ratio under respective flow conditions. The r_ζ/r_κ ratios thus obtained under extension and shear were found to exhibit the same dependence on the Weissenberg number Wi , given that Wi was reduced to an *iso*-local stretch state wherein the local elastic unit of the chain (Rouse spring) is stretched to the same extent under extension and shear. The analytical expressions of the rheological properties also enabled a preliminary test

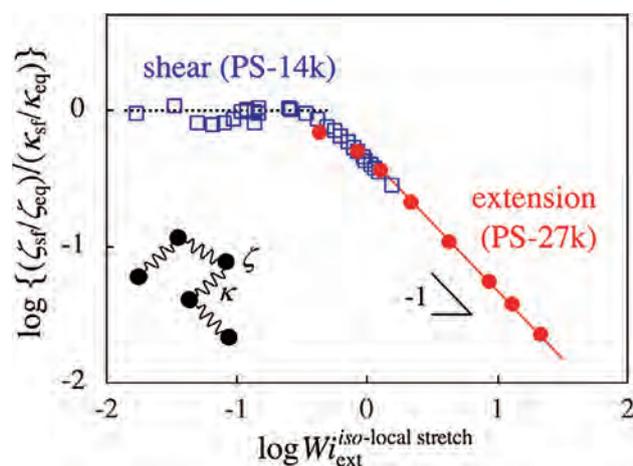


Figure 1. Comparison of the ratio of friction reduction factor ζ_{sf}/ζ_{eq} and spring strength reduction factor κ_{sf}/κ_{eq} against extensional Weissenberg number in the *iso*-local stretch condition Wi^{iso-lu} for PS-14k under shear and PS-27k under extension.

of the behavior of r_B . This test, made for the η_E , η_E^- , η , and Ψ_1 data mentioned above, posed a serious question about the relationships under fast flow often assumed in molecular models, $r_B = r_\zeta$ (proportionality between B and ζ not affected by flow) and $r_B = 1$ (no flow effect on B).

Viscoelastic and Dielectric Behavior of Polyisoprene Monofunctionally Head-Modified with Associative Metal-carboxylate Group

For moderately entangled high-*cis* polyisoprene (molecular weight = 30.5×10^3) head-modified with an associative metal-carboxylate (salt) group, PI30-COOM with $M = \text{Li, Na, and K}$, linear viscoelastic and dielectric measurements were conducted to examine an effect(s) of the head-to-head association on the chain dynamics. The PI30-COOM chains had type-A dipoles so that their large-scale dynamics was reflected in both viscoelastic and dielectric data at low angular frequencies. The salt groups associate and dissociate (without ionization) with a rate that changes with the temperature T , as known for ionomers having non-polar backbones. Correspondingly, PI30-COOM exhibited failure of the time-temperature superposition for both viscoelastic and dielectric data. This failure was characterized through comparison with non-associative reference homo-PI, the PI30 unimer (a precursor of PI30-COOM), (PI30)₂ dimer, and (PI30)₆ star-type hexamer. It turned out that the viscoelastic data of PI30-COOLi at low and intermediate T (-20° and 20°C), respectively, were close to those of the star-hexamer and dimer data in the *iso*-frictional state, and a further increase of T resulted in deviation from the dimer data toward the unimer data. This “crossover” was observed also for PI30-COONa and PI30-COOK but at lower T , which possibly reflected a barrier for the dissociation of the COOM groups lowering in the order of COOLi > COONa > COOK. The dielectric data of PI30-COOM showed a qualitatively similar crossover but at higher T compared to the viscoelastic crossover. This difference between the viscoelastic and dielectric behavior was discussed in relation to the dynamic tube dilation mechanism and also to the motional coupling (conformational transfer) among the PI30-COOM chains coexisting in different association forms.

Division of Multidisciplinary Chemistry – Molecular Aggregation Analysis –

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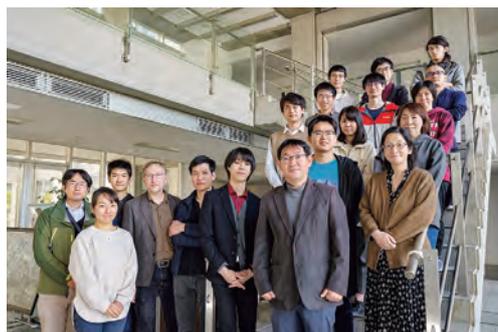
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Scope of Research

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



Recent Selected Publications

Jegorovė, A.; Truong, M. H.; Murdey, R.; Daskeviciene, M.; Malinauskas, T.; Kantminiene, K.; Jankauskas, V.; Getautis, V.; Wakamiya, A., Starburst Carbazole Derivatives as Efficient Hole Transporting Materials for Perovskite Solar Cells, *Sol. RRL.*, **6**, 2100877 (2021).
Hu, S.; Truong, M. H.; Otsuka, K.; Handa, T.; Yamada, T.; Nishikubo, R.; Iwasaki, Y.; Saeki, A.; Murdey, R.; Kanemitsu, Y.; Wakamiya, A., Mixed Lead-Tin Perovskite Films with >7 μ s Charge Carrier Lifetimes Realized by Maltol Post-Treatment, *Chem. Sci.*, **12**, 13513-13519 (2021).
Cho, Y.; Kim, H. D.; Zheng, J.; Bing, J.; Li, Y.; Zhang, M.; Green, M. A.; Wakamiya, A.; Huang, S.; Ohkita, H.; Ho-Baillie, A. W. Y., Elucidating Mechanisms behind Ambient Storage-Induced Efficiency Improvements in Perovskite Solar Cells, *ACS Energy Lett.*, **6**, 925-933 (2021).
Truong, M. H.; Lee, H.; Shimazaki, A.; Mishima, R.; Hino, M.; Yamamoto, K.; Otsuka, K.; Handa, T.; Kanemitsu, Y.; Murdey, R.; Wakamiya, A., Near-Ultraviolet Transparent Organic Hole-Transporting Materials Containing Partially Oxygen-Bridged Triphenylamine Skeletons for Efficient Perovskite Solar Cells, *ACS Appl. Energy Mater.*, **4**, 1484-1495 (2021).

Near-ultraviolet Transparent Organic Hole-Transporting Materials Containing Partially Oxygen-bridged Triphenylamine Skeletons for Efficient Perovskite Solar Cells

Organic semiconducting materials that are optically transparent in the near-ultraviolet (NUV) region from 300 to 400 nm are needed for advanced perovskite devices such as bifacial semitransparent and tandem solar cells. In this study, three organic semiconducting materials, **HND-NAr₂**, **HND-DTP**, and **HND-Cbz**, were designed and synthesized by introducing bis(4-methoxyphenyl)amine, dithieno[3,2-b:2',3'-d]pyrrole, and carbazole, respectively, into the head position of partially oxygen-bridged triphenylamine skeletons. The combination of oxygen-bridged triphenylamine and an electron-donating group at the head position suppresses the π - π^* transition, leading to weak absorption in the NUV region. Thin films of the materials can be fabricated by both solution and vacuum-deposition processes, and applied as the hole-transporting material (HTM) in perovskite solar cells (PSCs). The power conversion efficiency (PCE) of conventional devices with these HTMs was 13.7 % (**HND-Cbz**), 15.0 % (**HND-DTP**), and 17.2 % (**HND-NAr₂**). When used in bifacial semitransparent PSCs, the incident photon-to-current conversion efficiency (IPCE) at 400 nm was 41 % (**HND-NAr₂**), 45 % (**HND-Cbz**), and 46 % (**HND-DTP**), significantly higher than that of a reference using 2,2',7,7'-tetrakis(N,N-di-p-methoxyphenylamine)-9,9'-spirobifluorene (spiro-OMeTAD) as the HTM (14 %) as a result of the improved optical transmission through the HTM.¹

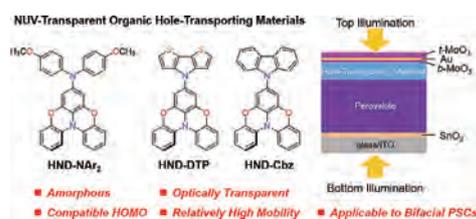


Figure 1. Chemical structures of NUV-transparent organic hole-transporting materials.

Mixed Lead–tin Perovskite Films with >7 μ s Charge Carrier Lifetimes Realized by Maltol Post-treatment

Mixed lead–tin (Pb–Sn) halide perovskites with optimum band gaps near 1.3 eV are promising candidates for next-generation solar cells. However, the performance of solar cells fabricated with Pb–Sn perovskites is restricted by the facile oxidation of Sn(II) to Sn(IV), which induces self-doping. Maltol, a naturally occurring flavor enhancer and strong metal binding agent, was found to effectively suppress Sn(IV) formation and passivate defects in mixed Pb–Sn perovskite films. When used in combination with Sn(IV) scavenging, the maltol surface treatment led to

high-quality perovskite films which showed enhanced photoluminescence intensities and charge carrier lifetimes in excess of 7 μ s. The scavenging and surface treatments resulted in highly reproducible solar cell devices, with photoconversion efficiencies of up to 21.4 % under AM1.5G illumination.²

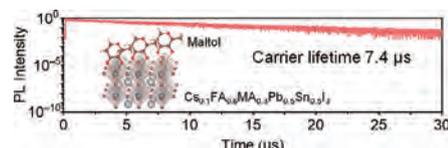


Figure 2. Ultralong charge carrier lifetime of lead-tin perovskite films realized by maltol post-treatment.

Materials Chemistry Approach for Efficient Lead-free Tin Halide Perovskite Solar Cells

The commercial development of perovskite-based photovoltaics is hindered by the toxicity of lead perovskite. Although tin perovskite is a promising alternative, the power conversion efficiency of tin perovskite solar cells has not reached levels comparable to the lead-based devices. Several factors, including the facile oxidation of tin(II) to tin(IV) and difficulties in controlling the morphology of the perovskite layers, are responsible for the lower efficiency. By closely integrating the development of high-purity materials and improved fabrication methods with extensive material characterization, we have been able to improve the performance of tin-based perovskite devices. In this work, highly purified precursor materials for tin perovskites are introduced, together with fabrication methods for pinhole-free and uniform tin perovskite films. The oxidation of tin(II) to tin(IV) during the fabrication process is suppressed by an in situ reducing treatment, which leads to tin perovskite films essentially free from tin(IV) impurities.³

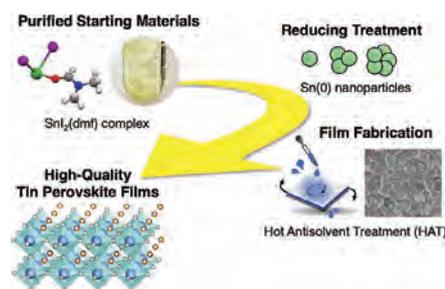


Figure 3. Schematic illustration of the materials chemistry approach for efficient tin halide perovskite solar cells.

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- 2) S. Hu, M. A. Truong, K. Otsuka, T. Handa, T. Yamada, R. Nishikubo, Y. Iwasaki, A. Saeki, R. Murdey, Y. Kanemitsu, A. Wakamiya*, *Chem. Sci.* **2021**, *12*, 13513.
- 3) T. Nakamura, T. Handa, R. Murdey, Y. Kanemitsu*, A. Wakamiya*, *ACS Appl. Electron. Mater.* **2020**, *2*, 3794.

Advanced Research Center for Beam Science – Particle Beam Science –

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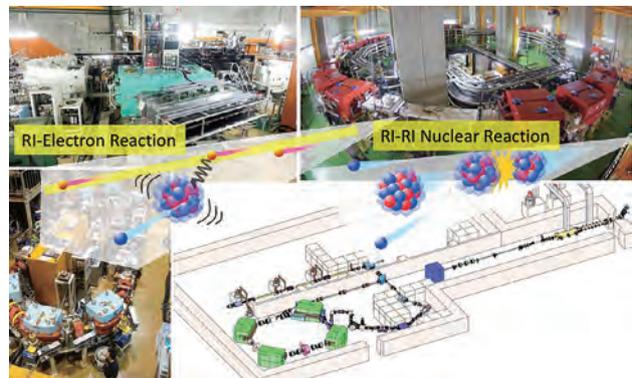
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Scope of Research

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	



Recent 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).
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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).

Development of Resonant-extraction Charge Breeder (RECB) for RUNBA

RUNBA (Recycled-Unstable-Nuclear Beam Accumulator) project aims at developing and establishing a beam recycling technique in a storage ring for nuclear reaction studies with rare RI ions. This project is addressed under the joint research program between ICR Kyoto University and RIKEN Nishina Center.

RI ions injected with the energy of 10 keV/u are accelerated to 10 MeV/u in RUNBA for nuclear reaction experiments. For an efficient acceleration, it is essential that RI ions are in highly charged state. Although an EBIT (Electron beam ion trap) type charge breeder (CB) is widely used to convert the singly charge state to the highly charge state, the efficiency has so far been around only 20 %. The low efficiency is fatal to research the rare-RI nuclear reaction. To improve the efficiency, we developed a novel type of CB named a resonant extraction charge breeder (RECB). Only desired charge state ions are selectively extracted from RECB with expecting the conversion efficiency of 100 %.

Ions injected to RECB are trapped by electrostatic potential with quadratic shape in the longitudinal direction and a large current of thin electron beam. The longitudinal motion of ions is a simple harmonic oscillation, and its frequency depends on the mass-to-charge ratio. Thus, when we oscillate the electro statistic potential at a certain frequency, the ions with a unique charge state are excited and they overcome the potential barrier. Then the ions of only a selected charge state are extracted from the RECB, and the others are left.

In this year, we tried proof-of-principle experiments of the RECB by using residual gas ions. Figure 1 shows some

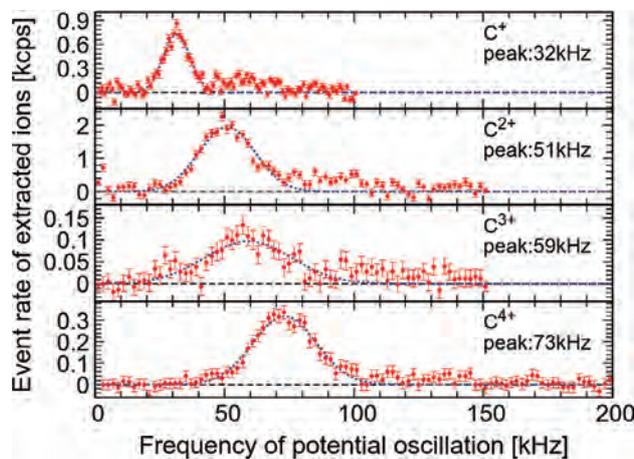


Figure 1. Event rate of extracted ions depended on a potential oscillation frequency in RECB.

examples of spectrum for extracted $^{12}\text{C}^{1-4+}$ ions. The $^{12}\text{C}^{1-4+}$ ions are extracted with the frequency of 32, 51, 59, 73 kHz, respectively. These results demonstrated the possibility of the charge-state-selectable extraction from RECB. In a future work, we will optimize the potential oscillation design to improve the frequency resolution.

Development of a Control System for KAKEN Accelerators

We have been developed a radiation management system (RMS) based on Experimental Physics and Industrial Control System (EPICS) for operating KAKEN Electron Linac (KEL) and KAKEN Storage Ring (KSR). A controller and I/O modules of the RMS are FA-M3 Programmable Logic Controllers (PLC, Yokogawa Electric Corp.). RMS core programs are ladder logic programs for personal protection systems (PPS), and EPICS Input Output Controllers (IOC) for an accelerator control, and a FPGA-based timing system for accelerator triggers using CompactRIO (National Instrument Corp.). Figure 2 shows an operation interface of KEL/KSR status monitor made by Control-System Studio (CSS). We plan to release the RMS and to drive the KEL and KSR during this year.

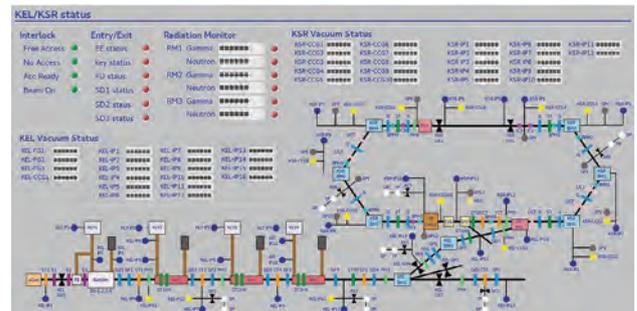


Figure 2. KEL/KSR status monitor made by CSS software.

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

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



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HASHIDA, Masaki
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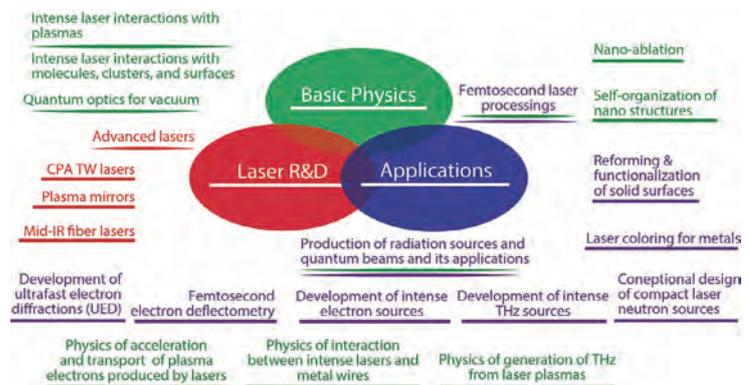
MASUNO, Shin-ichiro (M Sc)

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



Recent Selected Publications

Takenaka, K.; Shinohara, N.; Hashida, M.; Kusaba, M.; Sakagami, H.; Sato Y.; Masuno, S.; Nagashima, T.; Tsukamoto, M., Delay Times for Ablation Rate Suppression by Femtosecond Laser Irradiation with a Two-Color Double-Pulse Beam, *Appl. Phys. Lett.*, **119**, 261603 (2021).
Kojima, S.; Miyatake, T.; Inoue, S.; Dinh, T. H.; Hasegawa, N.; Mori, M.; Sakaki, H.; Nishiuchi, M.; Dover, N. P.; Yamamoto, Y.; Sasaki, T.; Ito, F.; Kondo, K.; Yamanaka, T.; Hashida, M.; Sakabe, S.; Nishikino, M.; Kondo K., Absolute Response of a Fuji BAS-TR imaging Plate to Low-energy Protons (<0.2 MeV) and Carbon Ions (<1 MeV), *Rev. Sci. Instrum.*, **92**, 033306 (2021).
Furukawa, Y.; Hashida, M.; Inoue, S., Temporal Change in Laser Penetration Length of Titanium and Platinum for Double-pulse Ablation Measured by a Novel Ablation Method, *J. Laser Appl.*, **33**, 012023 (2021).
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).
Hosokawa, C.; Hashida, M.; Nagashima, T.; Inoue, S.; Sakabe, S., Development of Intense Terahertz Light Source for Forming Periodic Structures on Material Surface, *IEEJ Trans. Fund. Materi.*, **140(8)**, 378-382, (2020).

Delay Times for Ablation Rate Suppression by Femtosecond Laser Irradiation with a Two-Color Double-Pulse Beam

We examined ablation rate suppression on a Ti surface for a delay time Δt between zero and 600 ps with a two-color femtosecond double-pulse laser beam. The double-pulse beam comprised cross-polarized pulses with 150-fs and >150 -fs pulse widths with 800-nm and 400-nm wavelengths, respectively. The ablation rate was clearly suppressed at the delay time of $\Delta t = 60$ ps with a 800-nm first pulse. With a 400-nm first pulse, the ablation rate was suppressed at the delay time of $\Delta t = 200$ ps. The delay time of greatest ablation suppression differed by a factor of approximately three between the two irradiation cases. The difference in the delay time of greatest ablation suppression suggests that the ablation rate was effectively suppressed when the expanding surface plasma produced by the first laser pulse was close to the critical density for the second laser pulse.

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 $F_{800th} = 0.108 \text{ J/cm}^2$ and $F_{400th} = 0.090 \text{ J/cm}^2$, respectively. We found that uniform LIPSSs could be produced on titanium surfaces using laser fluences of $1.5F_{400th} + 0.9F_{800th}$ 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.

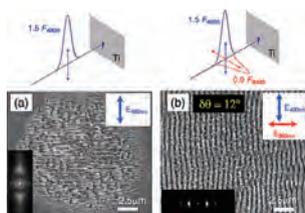


Figure 1. SEM images of titanium surfaces irradiated with (a) only the fundamental wavelength pulse with $N = 60$ pulses and (b) the two-color double-pulse beam with delay of $\Delta t = 0$ and $N = 60$ pairs of pulses. The LIPSS uniformity ($\delta\theta$) shows LIPSS characterized by the 800 nm pulse.

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.

Advanced Research Center for Beam Science – Electron Microscopy and Crystal Chemistry –

<http://eels.kuicr.kyoto-u.ac.jp/EMCC/home-en.html>



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Students

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IWASHIMIZU, Chisaki (D2) KAZAMA, Hiroki (M1)

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 Core-Hole First-Principle Calculation

Recent Selected Publications

Haruta, H.; Nii, A.; Hosaka, Y.; Ichikawa, N.; Saito, T.; Shimakawa, Y.; Kurata, H., Extraction of the Local Coordination and Electronic Structures of FeO₆ Octahedra Using Crystal Field Multiplet Calculations Combined with STEM-EELS, *Appl. Phys. Lett.*, **117**, [132902-1]-[132902-5] (2020).

Yamaguchi, A.; Nemoto, T.; Kurata, H., Study of C K-Edge High Energy Resolution Energy-Loss Near-Edge Structures of Copper Phthalocyanine and Its Chlorinated Molecular Crystals by First-Principles Band Structure Calculations, *J. Phys. Chem. A*, **124**, 1735-1743 (2020).

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).

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., Atomic-Resolution Two-Dimensional Mapping of Holes in the Cuprate Superconductor La_{2-x}Sr_xCuO_{4±δ}, *Physical Review B*, **97**, [205139-1]-[205139-5] (2018).

Study of C K-Edge High Energy Resolution Energy-Loss Near-Edge Structures of Copper Phthalocyanine by First-Principles Band Structure Calculations

While electron energy-loss spectroscopy combined with scanning transmission electron microscopy (STEM-EELS) is powerful tool for high spatial resolution elemental and state analyses, it has not been used very often for organic crystals because of problems with radiation damage to the specimen and poor energy resolution. However, these problems can be partly overcome by a reduction of the acceleration voltage and the incorporation of a monochromator into the electron gun. On the other hand, energy-loss near-edge structure (ELNES) spectrum for organic crystals is often interpreted by using molecular orbital (MO) method. However, first-principles band structure calculation is necessary to include the effect of core-hole. In the present study, we aim to interpret C K-edge ELNES measured from copper phthalocyanine (CuPc) crystals using monochromated STEM-EELS by first-principles band structure calculation including a core-hole.

There are four nonequivalent carbon atoms in the molecule; therefore, it is necessary to calculate the spectrum by the introduction of a core-hole at each nonequivalent carbon site (C1, C2, C3, C4). Figure 1 shows the C K-edge ELNES spectra measured for CuPc. The calculated spectra based on the ground state (GS), half core-hole state, and full core-hole state calculations are also presented in this figure. The half core-hole calculation result is most consistent with the experimental result in terms of the spectral shape and the relative intensity of each peak. This suggests that the core-hole potential in conjugate molecules is relatively well screened due to the delocalized π -electrons. Figure 2 shows the PDOSs with p-symmetry of each nonequivalent carbon site in the GS and the half core-hole states to assign each peak in the ELNES spectrum. It is noted that the PDOSs consist of isolated narrow distributions with widths of ca. 0.5 eV, which means that the band dispersion is small and the intermolecular interaction is weak and is consistent with MO method. The introduction of half a core-hole causes the PDOS to be shifted uniformly to the low energy side by ca. 0.6 eV, except for the peaks marked with an asterisk, which indicates the stabilization of electronic states by the potential of the core-hole. Figure 3 shows spatial distributions of the isolated states within a specific energy range in the PDOS of the half core-hole state. The distribution is susceptible to the core-hole effect. Although such site-dependent core-hole effects have already been pointed out in the previous study by MO calculations, we can confirm a similar core-hole effect in terms of the PDOS and the spatial distribution of unoccupied states with half a core-hole obtained from the all-electron first-principles band structure calculation.

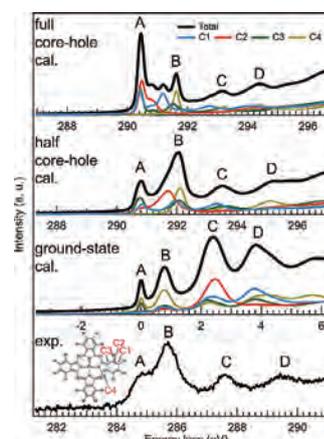


Figure 1. Experimental C K-edge ELNES spectrum of CuPc compared with the calculated spectra of the ground state, half core-hole state, and full core-hole state. The contributions of each carbon site are superimposed in the calculated spectra.

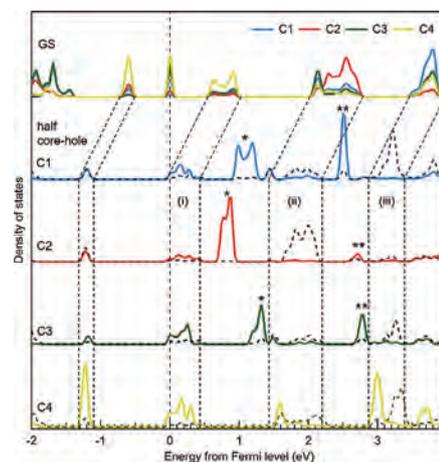


Figure 2. PDOSs with p-symmetry at four nonequivalent carbon sites of CuPc in the GS and the half core-hole state. The PDOSs of the half core-hole state at core-hole sites and its equivalent sites without a core-hole are shown by solid and dashed lines, respectively.

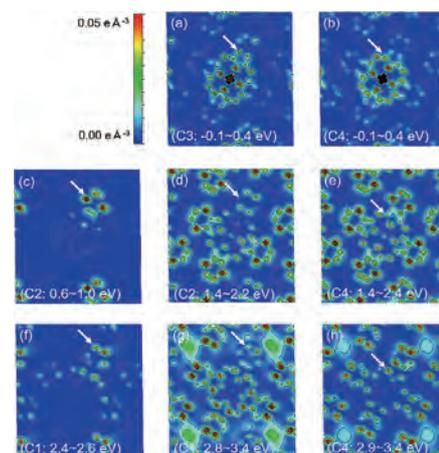


Figure 3. Spatial distributions of the isolated states within a specific energy range in the PDOS of the half core-hole state of CuPc. The arrow indicates the carbon site introducing half a core-hole.



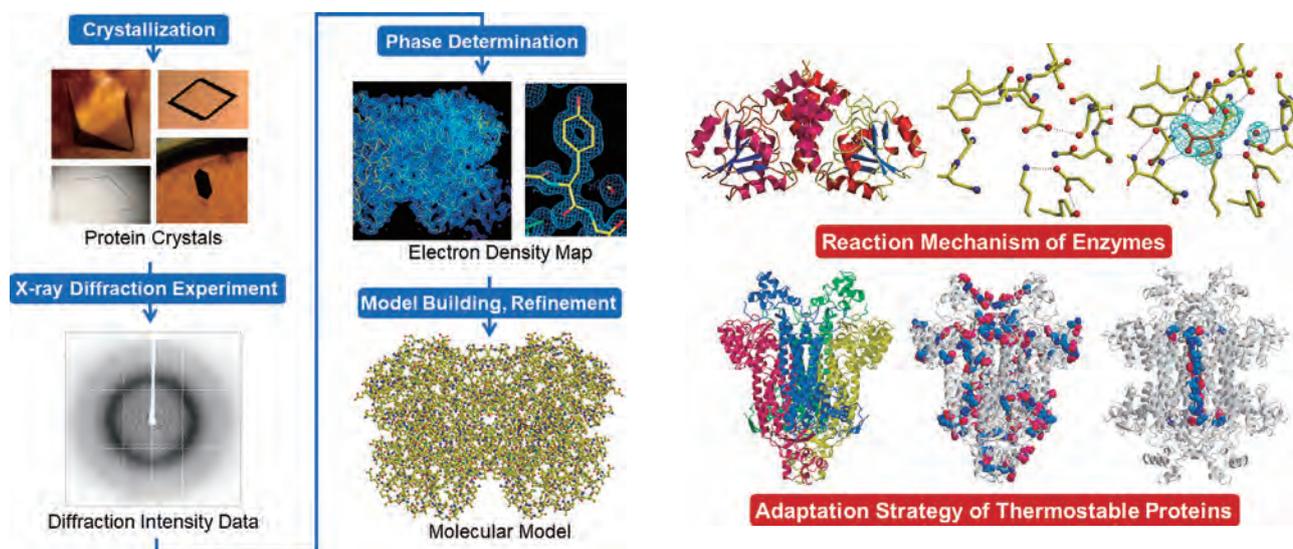
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FUJII, Tomomi
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Scope of Research

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



Recent Selected Publications

- Fujii, T.; Sato, A.; Okamoto, Y.; Yamauchi, T.; Kato, S.; Yoshida, M.; Oikawa, T.; Hata, Y., The Crystal Structure of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005 Provides Insights into the Reaction Mechanism of Enzymes in Its Original Family, *Proteins: Structure, Function, and Bioinformatics*, **84**, 1029-1042 (2016).
- Fujii, T.; Yamauchi, T.; Ishiyama, M.; Gogami, Y.; Oikawa, T.; Hata, Y., Crystallographic Studies of Aspartate Racemase from *Lactobacillus sakei* NBRC 15893, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **71**, 1012-1016 (2015).
- Fujii, T.; Goda, Y.; Yoshida, M.; Oikawa, T.; Hata, Y., Crystallization and preliminary X-ray Diffraction Studies of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **64**, 737-739 (2008).
- Fujii, T.; Oikawa, T.; Muraoka, I.; Soda, K.; Hata, Y., Crystallization and Preliminary X-ray Diffraction Studies of Tetrameric Malate Dehydrogenase from the Novel Antarctic Psychrophile *Flavobacterium frigidimarum* 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 GraC from *Rhizobium* sp. Strain MTP-10005 in Complex with Coenzyme and Ligand

Rhizobium is a genus of tubercle-forming bacteria. It grows in symbiosis with the root of a plant to fix nitrogen from the air. Although considerable attention has been paid to *Rhizobium* genes and gene products, there is still little information available on the molecular structures, functions, and properties of the enzymes involved in the metabolic pathways. *Rhizobium* sp. strain MTP-10005 was isolated from natural river water during a screening experiment. Enzymological and genetic studies showed that the translational products of the *graA*, *graB*, *graC*, and *graD* genes (GraA, GraB, GraC, and GraD, respectively) could be potentially involved in the resorcinol degradation pathway. To reveal the structure and function of all these proteins, we have performed X-ray structural studies of the proteins. In this study, we focused on maleylacetate reductase (GraC), which catalyzes the NADH- or NADPH-dependent reduction of maleylacetate to 3-oxoadipate and attempted to determine the structure of GraC-cofactor-ligand complex.

The GraC-NADH complex crystals were prepared using the sitting-drop vapor-diffusion method with a protein solution containing NADH and a reservoir solution containing PEG1500. The crystals were soaked in cryoprotectant solutions containing PEG1500, NADH, and each of several substrate analogs. Each soaked crystal was picked up in a cryoloop and frozen immediately in liquid nitrogen. Diffraction experiments were performed at Photon Factory, KEK, Japan. Diffraction data for each crystal were collected under cryogenic conditions. The electron density maps were calculated using the data collected for each crystal and the phases derived from the previously determined structural model of the GraC-NADH complex. The electron density map of the crystal soaked in the cryoprotectant solution containing 10 mM adipic acid dipotassium salt showed a blob of density at the active site. An adipate molecule was modeled in the blob, and the structure was refined at 1.9 Å resolution.

In the present crystal, one homodimeric GraC molecule exists in the *P1* unit cell. Each subunit binds one NADH molecule, while only one subunit binds one adipate molecule (Figure 1). The subunit of GraC molecule consists of two domains: an N-terminal domain with an α/β structure formed by residues 1–159 and a C-terminal α -helical domain formed by residues 160–351. The adipate molecule is located in the vicinity of NADH bound to the active site cleft between the domains of the subunit (Figure 2). The superposition of subunit C α atoms between GraC-NADH-

adipate and GraC-NADH complexes results in the root mean square deviations of 0.49 Å. No significant conformational changes are observed in the protein backbone upon the binding of adipate to the GraC-NADH complex. In the active site, one of the carboxyl groups of the adipate molecule forms hydrogen bonds with the side-chains of Asn170, His243, His253, and His257. These residues might be involved in substrate binding or catalysis (Figure 3).



Figure 1. Dimeric molecular structure of GraC-coenzyme-ligand complex.

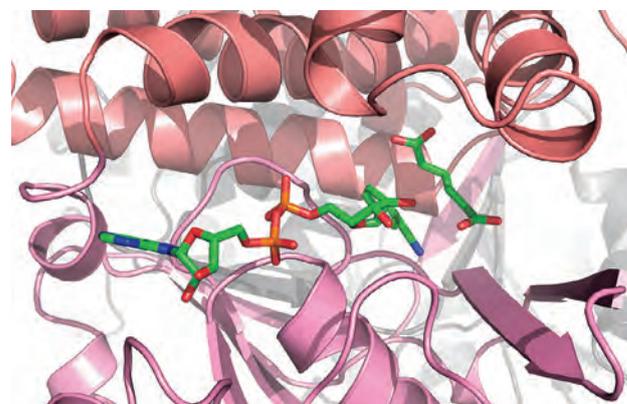


Figure 2. The active-site cleft of GraC-coenzyme-ligand complex.

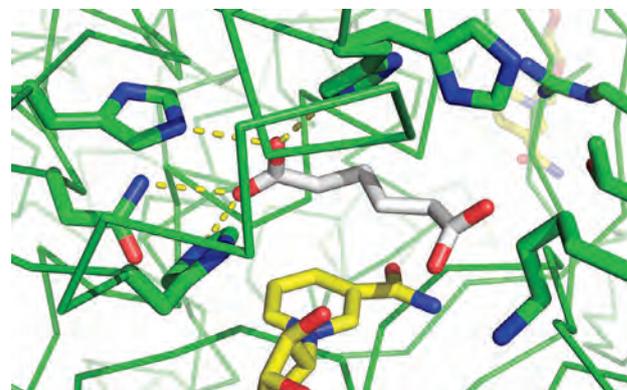


Figure 3. The active-site structure of GraC-coenzyme-ligand complex.

International Research Center for Elements Science – Synthetic Organotransformation –

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



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AVENA, Ramon Francisco Bernardino

Assist Techn Staff

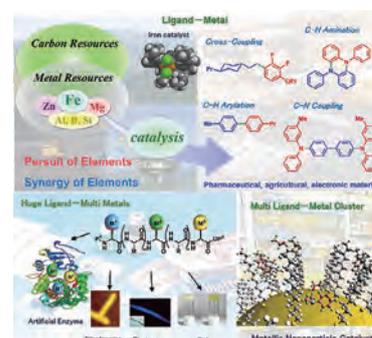
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Scope of Research

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

Synthetic Organic Chemistry Iron Catalysis Supramolecular Catalysis Metal Nanocluster Woody Biomass

Recent Selected Publications

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

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

Iwamoto, T.; Okuzono, C.; Adak, L.; Jin, M.; Nakamura, M., Iron-Catalysed Enantioselective Suzuki-Miyaura Coupling of Racemic Alkyl Bromides, *Chem. Commun.*, **55**, 1128-1131 (2019).

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

Adak, L.; Kawamura, S.; Toma, G.; Takenaka, T.; Isozaki, K.; Takaya, H.; Orita, A.; Li, H. C.; Shing, T. K. M.; Nakamura, M., Synthesis of Aryl C-Glycosides via Iron-Catalyzed Cross Coupling of Halosugars: Stereoselective Anomeric Arylation of Glycosyl Radicals, *J. Am. Chem. Soc.*, **139**, 10693-10701 (2017).

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 a recent representative example, we developed the iron-catalyzed enantioselective carbometalation of azabicycloalkenes (Figure 1a), which is of significant interest due to the facile installation of four stereocenters retaining the azabicyclic skeleton. By the combination of X-ray absorption spectroscopy and DFT calculation, we proposed a catalytic cycle of diaryliron complex involving coordination of azabicyclic alkene, olefin insertion, and transmetalation steps (Figure 1b).

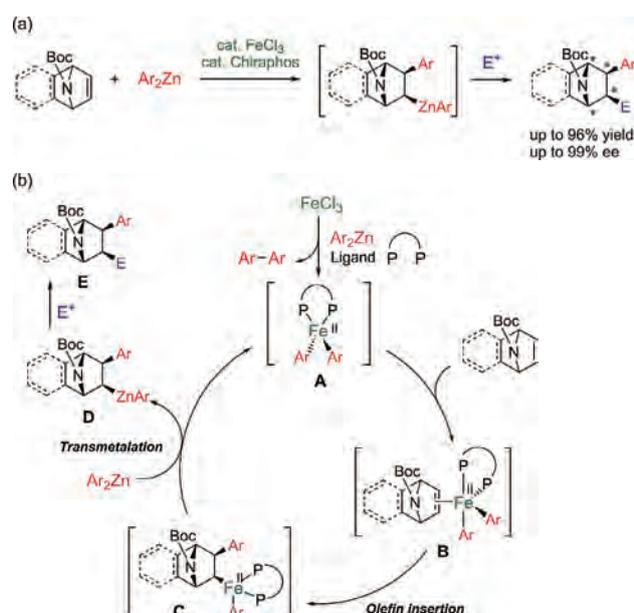


Figure 1. Iron-catalyzed enantioselective carbometalation of azabicycloalkenes. (a) General reaction scheme and (b) proposed catalytic cycle.

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 methoxybenzene 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. As a recent representative example, we reported the supramolecular reaction field effect of peptide dendron thiolate ligands on Au₂₅ nanocluster accelerating the photocatalytic oxidation of amino alcohols through the intermolecular interaction between peptide dendrons and substrates. The supramolecular reaction field effect was demonstrated by the 21 times faster conversion of amino alcohols to oxazolidine derivatives with peptide dendron thiolate ligands than that with conventional alkyl thiolate ligands.

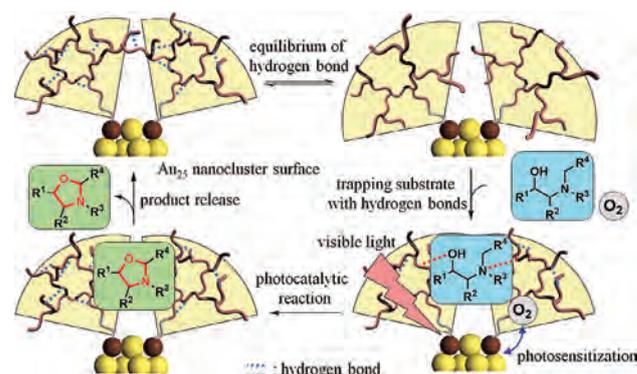


Figure 2. Schematic illustration of photocatalytic oxidation of amino alcohol accelerated by supramolecular reaction field constructed of peptide dendron thiolates on Au₂₅ nanocluster.

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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 Metal Oxides
High Pressure Synthesis Epitaxial Thin Film Growth
Heterointerface



Recent Selected Publications

- Goto, M.; Oguchi, T.; Shimakawa, Y., Geometrical Spin Frustration and Monoclinic-Distortion-Induced Spin Canting in the Double Perovskites $\text{Ln}_2\text{LiFeO}_6$ ($\text{Ln} = \text{La}, \text{Nd}, \text{Sm}, \text{and Eu}$) with Unusually High Valence Fe^{5+} , *J. Amer. Chem. Soc.*, **143**, 19207 (2021).
- Kosugi, Y.; Goto, M.; Tan, Z.; Kan, D.; Isobe, M.; Yoshii, K.; Mizumaki, M.; Fujita, A.; Takagi, H.; Shimakawa, Y., Giant Multiple Caloric Effects in Charge Transition Ferrimagnet, *Sci. Rep.*, **11**, 12682 (2021).
- Kan, D.; Suzuki, I.; Shimakawa, Y., Tuning Magnetic Anisotropy by Continuous Composition-Gradients in a Transition Metal Oxide, *J. Appl. Phys.*, **129**, 183902 (2021).
- Injac, S. D. A.; Xu, Y.; Romero, F. D.; Shimakawa, Y., Pauli-Paramagnetic and Metallic Properties of High Pressure Polymorphs of BaRhO_3 Oxides Containing Rh_2O_6 , *Dimers Dalton Trans.*, **50**, 4673 (2021).
- Tan, Z.; Koedtruid, A.; Goto, M.; Iihoshi, M.; Shimakawa, Y., Layered Hexagonal Perovskite Oxides $21\text{R Ba}_7\text{Fe}_3\text{Ge}_2\text{O}_{20}$ and $12\text{H Ba}_6\text{Fe}_3\text{Ge}_3\text{O}_{17}$, *Inorg. Chem.*, **60**, 1257 (2021).

Colossal Barocaloric Effect by Large Latent Heat Produced by First-Order Intersite-Charge-Transfer Transition

Solid thermomaterials are attracting much attention because they can be used to make innovative energy systems. An especially important application of thermomaterials is refrigeration technology. Materials showing large latent heat can be regarded as solid caloric effect materials, where entropy changes significantly in response to external fields, and they can be used to provide more efficient refrigeration than conventional refrigeration systems. They also eliminate the need for hydrofluorocarbon refrigerants, which are widely used in vapor-compression refrigeration but are linked to global warming. Candidate materials showing solid state caloric effects have been extensively explored. Typical solid-state caloric effects induced by magnetic fields, electric fields, and pressure are, respectively, called magnetocaloric, electrocaloric, and barocaloric effects. The magnetocaloric effects in solids, where a magnetic entropy difference between ferro- and para-magnetic spin alignments is produced by an external magnetic field, have been intensively studied for decades. Very recently, plastic crystals were reported to show colossal barocaloric effects. The exploration of new caloric materials is therefore accelerating.

We found in this study that the A-site-ordered quadruple perovskite-structure oxide $\text{NdCu}_3\text{Fe}_4\text{O}_{12}$ shows a colossal latent heat of 25.5 kJ/kg (157 J/cc), which corresponds to a large entropy change of 84.2 J/K·kg, produced by an intersite charge-transfer (CT) transition occurring near room temperature (Figure 1). The transition is first-order and is accompanied by an unusual magnetic ordering, not caused by simple magnetic interactions between spins, and a large negative-thermalexpansion-like volume change. We also demonstrated that the large latent heat is utilized through a barocaloric effect. The observed entropy change of 65.1 J/K·kg at 5.1 kbar is much larger than those reported in known giant barocaloric materials and is comparable to the largest changes reported in inorganic solid materials. The results point to $\text{NdCu}_3\text{Fe}_4\text{O}_{12}$ as a candidate material for

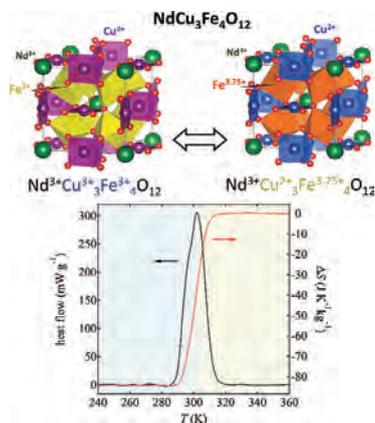


Figure 1. Crystal structure and valence states in high and low temperature phases of $\text{NdCu}_3\text{Fe}_4\text{O}_{12}$. DSC curve and Corresponding entropy change ΔS near room temperature measured during cooling.

use in thermal energy storage and refrigeration through the barocaloric effect.

Perpendicular Magnetic Tunnel Junctions Based on Half-Metallic NiCo_2O_4

Magnetic tunnel junctions (MTJs) with perpendicular magnetic anisotropy (PMA) have been regarded as an imperative component for next-generation high-density non-volatile memory devices. The tunnel magnetoresistance (TMR) ratio in MTJs is closely tied with spin polarization of conduction carriers in magnetic electrodes. Actually, MTJs composed of half-metals whose conduction carriers are fully spin-polarized (100 % spin polarization) have been reported to show large TMR ratios. Therefore, exploring magnetic materials that have high spin polarization as well as sufficient perpendicular magnetic anisotropy (PMA) is crucial for further developing perpendicular MTJs.

The inverse-spinel NiCo_2O_4 (NCO), in which the T_d -site is populated by Co, and the O_h -site is occupied by Ni and Co evenly, is a ferrimagnetic metal with a transition temperature above 400K and saturated magnetization of 1.5–2 m_B per formula unit (f.u.) [Figure 2]. Compressively strained epitaxial films of NCO (grown on MgAl_2O_4 substrates) have also been revealed to possess PMA, whose anisotropy energy is as large as 0.2 MJ/m³ at room temperature. Theoretical calculations indicated that the density of states at the E_F consists of only the minority-spin sub-band, leading to the half-metallic band structure with the spin polarization of -100 %. These observations imply that NCO is a candidate material that has both high spin polarization and sufficient perpendicular magnetic anisotropy, highlighting its potential application for spintronic devices.

Here, we show that all-oxide perpendicular MTJs, consisting of NCO as magnetic electrodes and the spinel oxide MgAl_2O_4 (MAO) as a tunnel barrier layer, have TMR ratios as large as 230 % under out-of-plane magnetic fields [Figure 2]. This result indicates that the spin polarization in perpendicularly magnetized NCO is as high as -73 %. Our experimental results demonstrate the potential of NCO as a half-metal with perpendicular magnetic anisotropy.

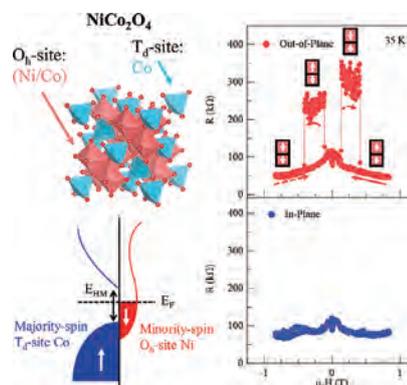


Figure 2. Crystal structure and schematic band diagram around the E_F of the inverse spinel oxide NiCo_2O_4 . Out-of-plane and in-plane magnetic field dependence of the $\text{NiCo}_2\text{O}_4/\text{MgAl}_2\text{O}_4/\text{NiCo}_2\text{O}_4$ junction resistance.

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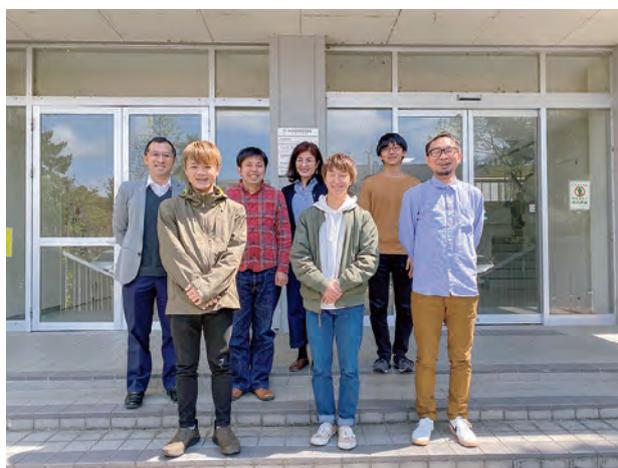
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Scope of Research

Developing efficient energy storage systems and innovative material production processes is a significant challenge for chemists to contribute to a sustainable society. We plan to approach these problems by using *transition metal clusters* of which multiple metal atoms work together as catalysts and functional materials. Our laboratory focuses explicitly on creating a new method to synthesize the clusters with atomic precision and applying the obtained clusters to difficult reactions such as the reduction of CO₂ and N₂.

KEYWORDS

Transition Metal Clusters
Homogeneous Catalysis
Nitrogen Fixation
Bioinorganic Chemistry



Recent Selected Publications

Wakioka, M.; Yamashita, N.; Mori, H.; Murdey, R.; Shimoaka, T.; Shioya, N.; Wakamiya, A.; Nishihara, Y.; Hasegawa, T.; Ozawa, F., Formation of *trans*-Poly(thienylenevinylene) Thin Films by Solid-State Thermal Isomerization, *Chem. Mater.*, **33**, 5631-5638 (2021).

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Tanifuji, K.; Jasnowski, A. J.; Villarreal, D.; Stiebritz, M. T.; Lee, C. C.; Wilcoxon, J.; Ohki, Y.; Chatterjee, R.; Bogacz, I.; Yano, J.; Kern, J.; Hedman, B.; Hodgson, K. O.; Britt, R. D.; Hu, Y.; Ribbe, M. W., Tracing the Incorporation of the “Ninth Sulfur” into the Nitrogenase Cofactor Precursor with Selenite and Tellurite, *Nat. Chem.*, **13**, 1228-1234 (2021).

Ohki, T.; Ishihara, K.; Yaoi, M.; Tada, M.; Sameera, W. M. C.; Cramer, R. E., A Dinuclear Mo₂H₈ Complex Supported by Bulky C₅H₂Bu₃ Ligands, *Chem. Commun.*, **56**, 8035-8038 (2020).

Ohki, Y.; Uchida, K.; Tada, M.; Cramer, R. E.; Ogura, T.; Ohta, T., N₂ Activation on a Molybdenum–Titanium–Sulfur Cluster, *Nat. Commun.*, **9**, 3200 (2018).

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

Biological N₂ fixation is conducted by nitrogenase that employs a unique Fe/Mo-S-C cluster as its catalytic site (FeMoco, [(*R*-homocitrate)MoFe₇S₉C]). Synthetic counterparts of the FeMoco, metal-sulfur clusters, demonstrated capturing N₂ on rare occasions; nevertheless, the catalytic conversion of this stable molecule has not been achieved despite its relevance to the biological N₂ fixation. This study focuses on capture, activation, and catalytic conversion of N₂ by an Fe atom incorporated into our [Mo₃S₄] incomplete-cubane platform bearing bulky Cp ligands. Treatment of these clusters with excess Na and ClSiMe₃ under a N₂ atmosphere gave N(SiMe₃)₃ with up to 248 eq. per cluster. This work exemplifies the N₂-reducing capability of Fe atoms in a S-rich environment, which biological systems have selected to achieve a similar purpose.

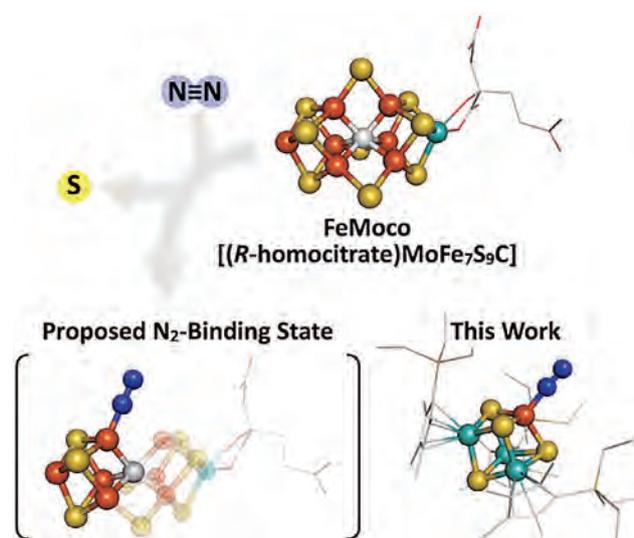


Figure 1. Proposed N₂ binding state of FeMoco and a N₂-bound Mo-Fe-S cluster.

Tracing the S Incorporation into the Nitrogenase Cofactor Precursor

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

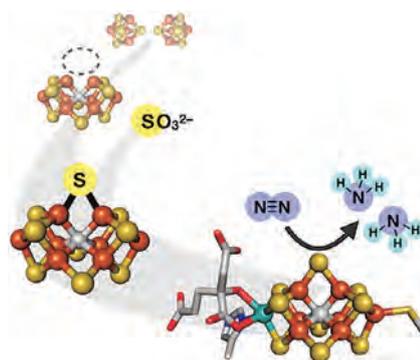


Figure 2. Schematic description of a sulfur uptake from sulfite (SO₃²⁻) in the biosynthetic pathway of FeMoco.

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Scope of Research

Our research interest is to understand optical and quantum properties of nanometer-structured materials and to establish opto-nanoscience for creation of innovative functional materials. Space- and time-resolved laser spectroscopy is used to study optical properties of semiconductor quantum nanostructures and strongly correlated electron systems in 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, 3) photophysics of solar cell materials, 4) engineering material properties with lights.



KEYWORDS

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

Recent Selected Publications

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

Halide-perovskite semiconductors are a promising material for future optoelectronic devices such as solar cells, and their excellent photocarrier properties are thought to originate from the characteristic electron-phonon interactions and phonon-mode characters. In this study, we explored the potential of THz pulses, which can resonantly excite the low-energy optical phonons, to modulate the photocarrier dynamics in $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite films. After THz pulse excitations, their impact on the photoinduced carrier dynamics was investigated by time-resolved photoluminescence (PL) spectroscopy. We observed the PL intensity was strongly modulated upon THz excitation in the picosecond time scale. Time-resolved PL spectra showed that the carrier temperature transiently increased, and furthermore, the PL intensity with high photon energies was enhanced by THz pulse excitation. These features indicate that the lifetime of hot carriers is enhanced by the phonon excitation induced by THz pulses, through the mechanism of hot-phonon bottleneck effect. These first observations suggest that the phonon systems, which are usually regarded as a passive heat bath, can be utilized as a new degree of freedom to efficiently harness photocarrier energy.

Ultrastrong Coupling between Phonons in Halide Perovskites and THz Vacuum Photons

When a matter is strongly coupled to the light field, a hybridized state emerges and behaves differently from the original electronic state. As the coupling strength increases, the hybrid system reaches the regime of ultrastrong coupling (USC). Especially, the USC between phonons and the vacuum field in a cavity is attracting much attention, because it opens up a novel way to material manipulation. However, this phononic USC remains difficult to achieve in solids because of the small dipole moments of phonon excitations. In our study, we found a way to increase coupling strength by enhancing the vacuum field, and thus realized the phononic USC. The system is made of the cavity of split ring resonator (SRR) and the phonon modes of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite semiconductor films at THz frequencies (Figure 1). Our analysis reveals that as the gap of SRR is narrowed, the enhancement of the vacuum field overcomes the decrease of the dipole number in a gap, finally resulting in the USC in a nano-size gap.

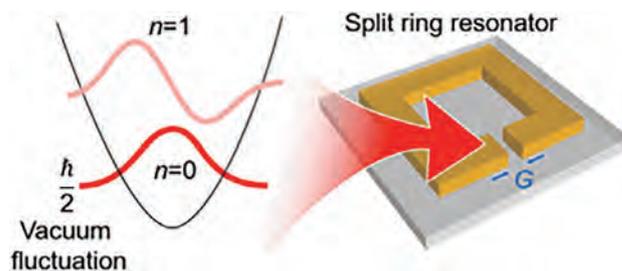


Figure 1. Image of vacuum field in a split ring resonator.

Size-dependent Exciton-phonon Coupling in Single Lead-halide Perovskite Nanocrystals

Lead-halide perovskite nanocrystals (NCs) are promising optical materials for use in several light-emitting devices. Recently, it has been reported that single perovskite NCs are suitable for single-photon sources because of their stable light emission and long exciton coherence time. In particular, exciton coherence time is strongly affected by the exciton-phonon coupling. To reveal the exciton-phonon coupling in perovskite NCs, we studied the NC size dependence of the PL spectra of FAPbX_3 (FA = $\text{HC}(\text{NH}_2)_2$, X = Br, I) NCs by using single-dot spectroscopy at liquid-helium temperature. We found four peaks below the exciton PL peak. By measuring size dependence of the PL peak energy and PL intensity, we concluded that they consist of two LO-phonon replicas of the exciton and emissions of charged exciton (trion) and biexciton (Figure 2). The binding energies of biexcitons and trions are size-dependent because of enhanced Coulomb interaction in smaller NCs. The LO-phonon energies are size-independent, but the strength of exciton-phonon coupling (the Huang-Rhys factors) becomes larger in smaller NCs. This phenomenon is probably due to the size-dependent dielectric constants and spatial separation of the electron and hole wavefunctions.

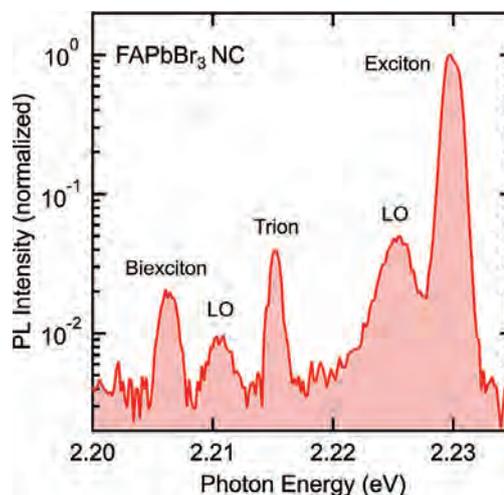


Figure 2. PL spectrum of a single perovskite nanocrystal.

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SHIH, Chi-Yu (Ph D) National Taiwan Ocean University, Taiwan, 23 August, 2021–31 July, 2022

Scope of Research

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



KEYWORDS

GenomeNet Bioinformatics Environmental Genomics Virology Molecular Evolution

Recent Selected Publications

Zhang, R.; Endo, H.; Takemura, M.; Ogata, H., RNA Sequencing of Medusavirus Suggests Remodeling of the Host Nuclear Environment at an Early Infection Stage, *Microbiol. Spectr.*, e0006421, doi: 10.1128/Spectrum.00064-21 (2021).

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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).

A Giant Virus Remodels the Host Nuclear Environment

Medusavirus, a recently isolated giant virus, has a nucleocytoplasmic replication cycle in amoebas during which the host nuclear membrane apparently remains intact, a unique feature among amoeba-infecting giant viruses. To investigate its infection strategy, we performed a time course RNA sequencing experiment. All viral genes were transcribed and classified into five temporal expression clusters. The immediate early genes (42 genes) were mostly (83 %) of unknown functions, frequently (95 %) associated with a palindromic promoter-like motif, and often (45 %) encoded putative nucleus-localized proteins. These results suggest massive reshaping of the host nuclear environment by viral proteins at an early stage of infection. Genes in the following clusters were assigned to various functional categories. The different expression profile between viral core histone genes and linker histone H1 gene suggests that they have distinct roles during the course of the virus infection. The transcriptional profile of the host *Acanthamoeba castellanii* genes was greatly altered postinfection. This work has been published in Zhang et al., *Microbiol. Spectr.*, 2021, doi: 10.1128/Spectrum.00064-21.

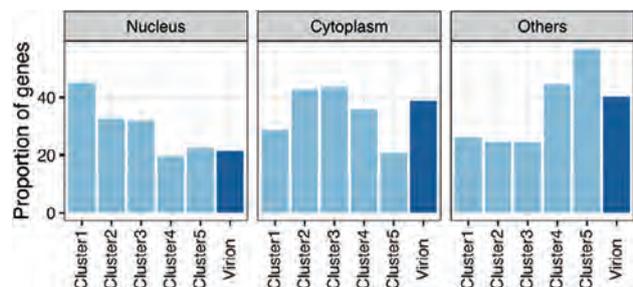


Figure 1. Predicted subcellular locations of viral proteins.

A Motor Protein Gene Discovered in Giant Viruses

Nucleocytoplasmic large DNA viruses (NCLDV) are a group of giant viruses. A typical phage particle is 150 nm and encapsulates a tens of thousands base pairs (bp) genome. In contrast, Mimivirus, a member of NCLDVs, is 750 nm in diameter and possesses a genome over 1,000 kbp. Although most of phage genes are essential for their replication and morphogenesis, NCLDVs sometimes encode genes, such as actin genes, that are apparently non-essential for their replication. In this study, we discovered myosin genes, named “virmyosin”, from NCLDV genomes. Our phylogenetic analysis revealed that some *Imitervirales* and *Phycodnaviridae* encode virmyosin. Especially, virmyosin-encoding *Imitervirales* are scattered in the phylogeny of *Imiternirales* family. Further investigation suggested that virmyosin of *Imitervirales* might have been recruited from marine plankton. Additional study showed an incongruence between the phylogenetic tree of NCLDVs and that of virmyosins, which suggested that horizontal gene transfers occurred not only between NCLDVs and eukaryotes but also between members of NCLDVs for the actin gene. We predicted the function of virmyosin in host cells based on previous studies. It has been known that myosins are motor proteins to walk along actin filaments, located at the peripheral side of cytoplasm. Some classes of myosin carry specific materials such as influenza virus. We thus consider that virmyosins may function as transporters of NCLDV particles. This work has been published in Kijima et al., *Front. Microbiol.*, 2021, doi: 10.3389/fmicb.2021.683294.

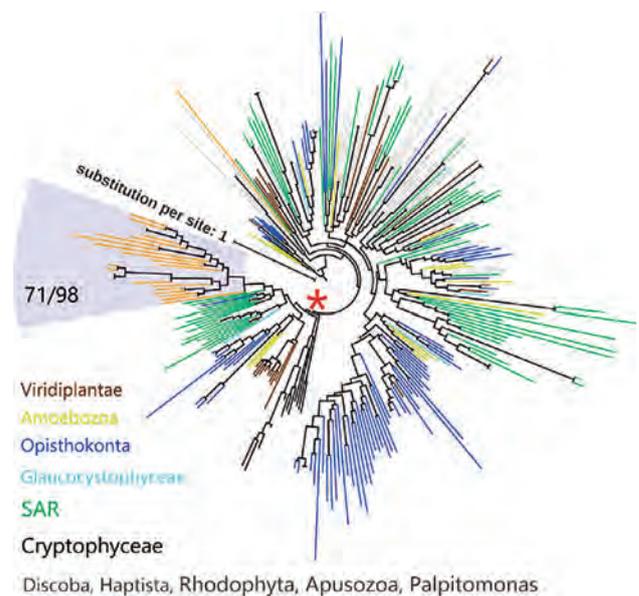


Figure 2. Phylogenetic tree of myosin genes of NCLDVs and eukaryotes, based on a maximum-likelihood framework. Color of each branch represents its taxonomic group (orange branches correspond to virmyosins).

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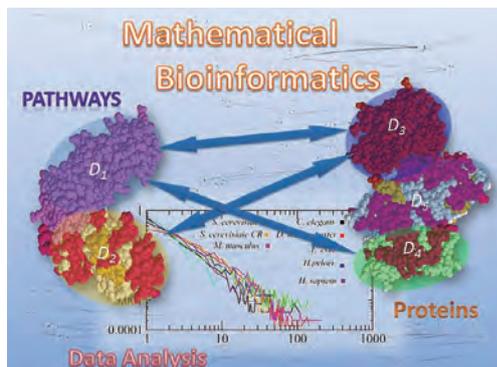
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TAKAGI, Motoshige (D3) NAKASHIMA, Shogo (D3) MA, Yier (M2)
LI, Ruiming (D3) MU, Lixuan (D2)
WANG, Feiqi (D3) SHIOTA, Koji (D1)

Scope of Research

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

KEYWORDS

Complex Networks
Boolean Networks
Neural Networks
Chemical Graphs
Protein Informatics



Recent Selected Publications

Akutsu T.; Jansson, J.; Li, R.; Takasu, A.; Tamura, T., New and Improved Algorithms for Unordered Tree Inclusion, *Theoretical Computer Science*, **883**, 83-98 (2021).
Cheng, C.; Ching, W-K.; Guo, S.; Akutsu, T., Discrimination of Attractors with Noisy Nodes in Boolean Networks, *Automatica*, **130**, 109630 (2021).
Nakajima, N.; Hayashi, T.; Fujiki, K.; Shirahige, K.; Akiyama, T.; Akutsu, T.; Nakato, R., Codependency and Mutual Exclusivity for Gene Community Detection from Sparse Single-Cell Transcriptome Data, *Nucleic Acids Research*, **49**, e104 (2021).
Kajiwara, M.; Nomura, R.; Goetze, F.; Kawabata, M.; Isomura, Y.; Akutsu, T.; Shimono, M., Inhibitory Neurons Exhibit High Controlling Ability in the Cortical Microconnectome, *PLoS Computational Biology*, **17**, e1008846 (2021).
Ma, Y.; Tamura, T., Dynamic Solution Space Division-based Methods for Calculating Reaction Deletion Strategies for Constraint-based Metabolic Networks for Substance Production, *Frontiers in Bioinformatics*, **1**, 716112 (2021).

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.

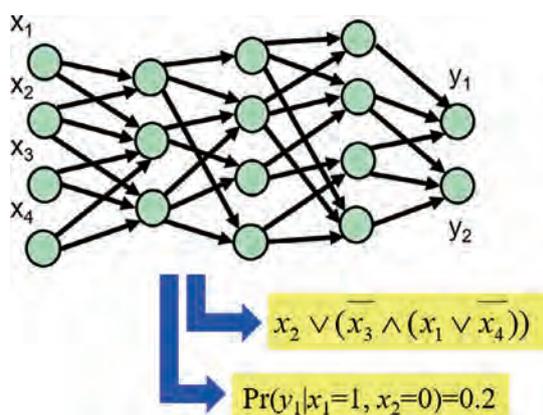


Figure 1. Our developed algorithms extract rules from trained neural networks in the forms of Boolean functions and conditional probabilities.

Gene Deletion Algorithms for Minimum Reaction Network Design by Mixed-integer Linear Programming for Metabolite Production in Constraint-based Models: gDel_minRN

Genome-scale constraint-based metabolic networks play an important role in the simulation of growth coupling, which means that cell growth and target metabolite production are simultaneously achieved. To achieve growth coupling, a minimal reaction-network-based design is known to be effective. However, the obtained reaction networks often fail to be realized by gene deletions due to conflicts with gene-protein-reaction relations.

Here, we developed gDel_minRN that determines gene deletion strategies using mixed-integer linear programming to achieve growth coupling by repressing the maximum number of reactions via gene-protein-reaction relations. Computational experiments were conducted in which gDel_minRN was applied to iML1515, a genome-scale model of *Escherichia coli*. The target metabolites were three vitamins that are highly valuable and require cost-effective bioprocesses for economics and the environment. gDel_minRN successfully calculated gene deletion strategies that achieve growth coupling for the production of biotin (vitamin B7), riboflavin (vitamin B2), and pantothenate (vitamin B5).

Since gDel_minRN calculates a constraint-based model of the minimum number of gene-associated reactions without conflict with gene-protein-reaction relations, it helps biological analysis of the core parts essential for growth coupling for each target metabolite. The source codes are implemented in MATLAB, CPLEX, and COBRA Toolbox. The obtained data and source codes are available on <https://github.com/taketam/gDel-minRN>

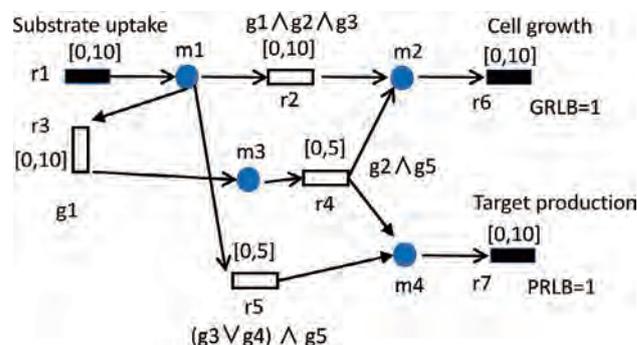


Figure 2. A toy example of the constraint-based model. Circles and rectangles represent metabolites and reactions, respectively. Black and white rectangles are external and internal reactions.

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)

Students

NGUYEN, Duc Anh (D3) NISHIKAWA, Emina (UG)

Guest Res Assoc

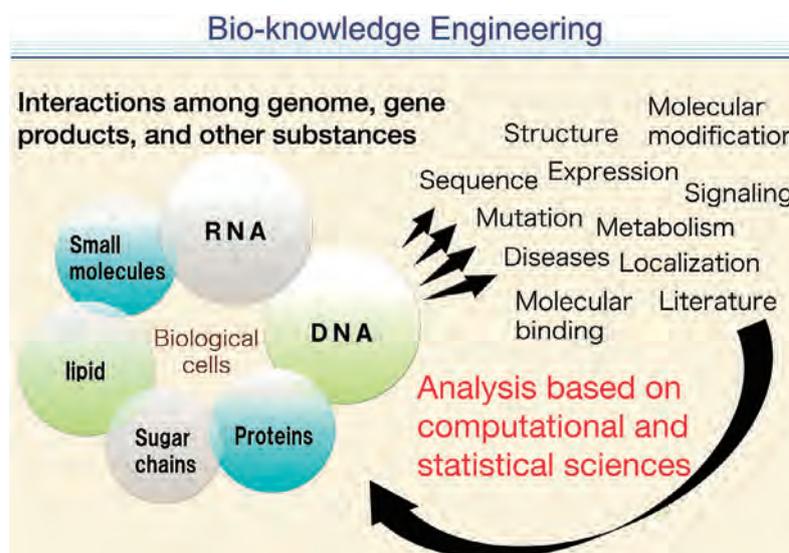
PETSCHNER, Peter (Ph D) Semmelweis University, Hungary, 28 November 2020– 27 November 2022

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



Recent Selected Publications

- Nguyen, C. H.; Mamitsuka, H., Learning on Hypergraphs with Sparsity, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, **43**, 2710-2722 (2021).
- Wimalawarne, K.; Mamitsuka, H., Reshaped Tensor Nuclear Norms for Higher Order Tensor Completion, *Machine Learning*, **110**, 507-531 (2021).
- You, R.; Yao, S.; Mamitsuka, H.; Zhu, S., DeepGraphGO: Graph Neural Network for Large-Scale, Multispecies Protein Function Prediction, *Bioinformatics*, **37**, I262-I271 (2021).
- 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, D. H.; Nguyen, C. H.; Mamitsuka, H., ADAPTIVE: Learning DATA-dePENDENT, Concise Molecular VECTORS for Fast, Accurate Metabolite Identification from Tandem Mass Spectra, *Bioinformatics*, **35(14)**, (Proceedings of the 27th International Conference on Intelligent Systems for Molecular Biology (ISMB/ECCB 2019)), i164-i172 (2019).

A Hypergraph Neural Network for Predicting Drug-drug Interactions

A drug-drug interaction (DDI) is a combination of two drugs causing side effects, which are unwanted reactions of human bodies. These side effects might be responsible for significant patient morbidity and mortality, and cost billions of dollars each year. Hence, predicting DDI is a very important task to guarantee drug safety in pharmacology. The traditional approach for predicting drug-drug interactions uses clinical trials on patients, which are time-consuming and costly. Recently, machine learning models have emerged as prominent tools for predicting DDI, which are fast and inexpensive.

Given drugs' information and known side effects of many pairs of drugs, one wishes to learn a model to predict side effects of all pairs of drugs. DDI is usually represented as a graph that nodes are drugs and edges are interacting drug pairs with side effects as labels. The task is to predict labels of all pairs of nodes in the DDI graph. Figure 1a shows an example DDI graph, where the dotted edge with question marks is the pair of drugs with labels to be predicted.

Existing work often uses graph neural networks to learn vector representations of drug nodes on the DDI graph and uses them to predict interactions. One drawback of this method is the lack of learning side effect representations. Side effects have complex relationships, for example, co-occurrences. Previous methods often represent each side effect as a one-hot vector indicating the presence of the side effect. This representation considers that side effects are independent, potentially under-utilizing the side effect relationships. Hence, it is necessary to learn representations of both side effects and drugs altogether.

To address the above drawback, we propose to encode DDI data with a hypergraph that a node in the hypergraph

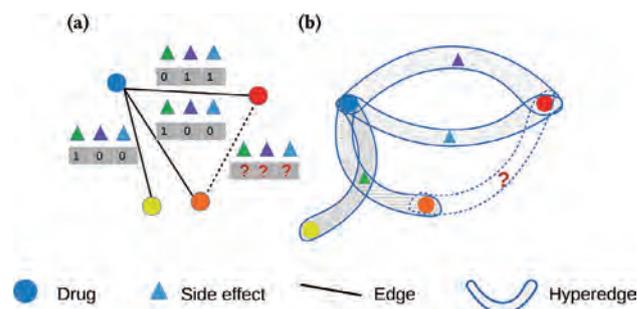


Figure 1. a) Traditional graph representation for DDI, b) Proposed hypergraph representation for DDI.

can be either a drug or a side effect and each hyperedge is a triple of two drugs and a side effect that they cause. Figure 1b illustrates an example of a hypergraph corresponding to the DDI graph in Figure 1a. We then propose CentSmoothie, a central-smoothing hypergraph neural network for predicting DDI, with a new assumption that in each hyperedge, the representation of the side effect node should be close to the midpoint of the corresponding subspace of the two drugs.

We conducted experiments on the benchmark DDI data to show the advantage of the prediction performance of our proposed method. We compared CentSmoothie with other state-of-the-art methods in terms of AUC (area under the ROC curve) and AUPR (area under the precision-recall curve). The results were shown in Figure 2. The results showed that our method (CentSmoothie) outperformed other methods in both AUC and AUPR, suggesting that our model was more suitable for DDI.

Reference

Duc Anh Nguyen, Canh Hao Nguyen, and Hiroshi Mamitsuka. "A survey on adverse drug reaction studies: data, tasks and machine learning methods." *Briefings in bioinformatics* 22, no. 1 (2021): 164-177.

Method	MLNN	MRGNN	Decagon	SpecConv	HPNN	CentSmoothie
AUC	0.8372 ± 0.0050	0.8452 ± 0.0036	0.8639 ± 0.0029	0.8785 ± 0.0025	0.9044 ± 0.0003	0.9348 ± 0.0002
AUPR	0.7919 ± 0.0041	0.8029 ± 0.0039	0.8094 ± 0.0024	0.8256 ± 0.0022	0.8410 ± 0.0007	0.8749 ± 0.0013

Figure 2. Performance comparison on the benchmark DDI data.



**HAKUBI RESEARCHERS’
ACTIVITIES IN ICR**

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



Research Topic

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



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.

Research Topic

Optoelectronic Energy Recycling and Quantum Cooperative Effects in Semiconductor Nanostructures



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

Host Laboratory Laboratory of Nanophotonics

Host Professor KANEMITSU, Yoshihiko

Outline of Research

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



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

iJURC Cooperative Research Subjects 2021

(1 April 2021 ~ 31 March 2022)

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

Synthesis and Optical Characterization of Gold Nanohelices with Controllable Aspect Ratio

NAKAGAWA, Makoto, Osaka Research Institute of Industrial Science and Technology

Host in iJURC KURATA, Hiroki

Development of Position Sensitive Active Target for Heavy Ion Storage Ring

YAMAGUCHI, Yoshitaka, RIKEN Nishina Center, Instrumentation Development Group

Host in iJURC WAKASUGI, Masanori

Verification of Radiochemical Reaction Mechanism for FLASH Radiotherapy with Electron Beams

KODAIRA, Satoshi, Radiation Measurement Group, Department of Radiation Measurement and Dose Assessment, National Institute of Radiological Sciences, National Institutes for Quantum Science and Technology

Host in iJURC OGAWARA, Ryo

Development of New Nano-structure Target for ISOL

OHNISHI, Tetsuya, RIKEN Nishina Center, SCRIT Team

Host in iJURC WAKASUGI, Masanori

Electronic Structure of Biomimetic $[\text{Mo}_3\text{S}_4\text{Fe}]$ Clusters and its Relation to the catalytic N_2 -Reduction: A Computational Study

SAMEERA, W. M. C., Institute of Low Temperature Science, Hokkaido University,

Host in iJURC OHKI, Yasuhiro

I

Gas Sensing Properties Research of Metal Oxides

GUO, Haichuan, Ningbo Institute of Industrial Technology (CNITECH) of the Chinese Academy of Sciences, China

Host in iJURC SHIMAKAWA, Yuichi

I

Investigating Iron Nitrides Prepared by New High-Pressure Synthesis with Mössbauer Spectroscopy

Kloß, Simon D., Centre for Science at Extreme Conditions and School of Chemistry, University of Edinburgh

Host in iJURC SHIMAKAWA, Yuichi

I

C-H Borylation and Silylation under Visible-Light Enabled Fe-Catalysis

HAJRA, Alakananda, Department of Chemistry, Visva-Bharati University

Host in iJURC NAKAMURA, Masaharu

I

Development of Iron-Based Electrocatalysts 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 Asymmetric Carbozincation and Ring-Opening Reactions of Oxabicyclic Alkenes

ADAK, Laksmikanta, Department of Chemistry, Indian Institute of Engineering Science and Technology

Host in iJURC NAKAMURA, Masaharu

I

Synthesis of Ferrocenyl-Phosphines and Their Application in the Preparation of Fe Clusters

OGASAWARA, Masamichi, Department of Natural Science, Graduate School of Science and Technology, Tokushima International Science Institute, and Research Cluster on "Innovative Chemical Sensing", Tokushima University

Host in iJURC OHKI, Yasuhiro

Development of THz-STM for Low-Temperature and High Magnetic Field

TACHIZAKI, Takehiro, Tokai University

Host in iJURC KANEMITSU, Yoshihiko

Strong Carrier Modulation in 2D Semiconducting Materials by Coupled Molecular Vibrations

KIRIYA, Daisuke, Osaka Prefecture University

Host in iJURC KANEMITSU, Yoshihiko

Exploration of Energy Materials by High Pressure Synthesis Technique

YABUUCHI, Naoaki, Department of Chemistry and Life Science, Yokohama National University

Host in iJURC KAN, Daisuke

Functionalization of Urushiol Coating Film Using Magnetic Particles

TACHIBANA, Yoichi, Kyoto Municipal Institute of Industrial Technology and Culture

Host in iJURC NAKAMURA, Masaharu

Development of Heteroacenes with Excellent Photophysical and Electrochemical Properties

MITSUDO, Koichi, Graduate School of Natural Science and Technology, Okayama University

Host in iJURC WAKAMIYA, Atsushi

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

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

Development of the Method for the Detection of Coronavirus Diversity

WATANABE, Tokiko, Research Institute for Microbial Diseases, Osaka University

Host in iJURC OGATA, Hiroyuki

Synthesis of Inorganic Molecules for Elucidation of Biosynthetic Pathways of Iron-Sulfur Clusters

RIBBE, Markus W., Department of Molecular Biology and Biochemistry, University of California, Irvine

Host in iJURC OHKI, Yasuhiro

I

I: International Joint Research

F: Female PI

Synthesis of Self-Assembled Organoboron Compounds, Elucidation of Self-Assembly Process, and Creation of New Functions
WAKABAYASHI, Shigeharu, Department of Clinical Nutrition, Faculty of Health Science, Suzuka University of Medical Science
Host in iJURC OHKI, Yasuhiro

Chiral Silica with Preferred-Handed Helical Structure via Chiral Transfer
HIRAI, Tomoyasu, Department of Applied Chemistry, Osaka Institute of Technology
Host in iJURC TAKENAKA, Mikihito

Elucidation of the Lubrication Properties of Hyperbranched Polymers and Their Optimization
TAKAHASHI, Yutaka, New Industry Creation Hatchery Center, Tohoku University
Host in iJURC TOSAKA, Masatoshi

Development of Simulation Scheme for Wall-Slip of Polymers
IANNIRUBERTO, Giovanni, Dipartimento di Ingegneria Chimica, dei Materiali e della Produzione Industriale, Università degli Studi di Napoli "Federico II"
Host in iJURC SATO, Takeshi I

Molecular Understanding on the Structures and Dynamics of End-Modified Polymers
VAO-SOONGNERN, Suranaree University of Technology
Host in iJURC WATANABE, Hiroshi I

Effect of Microplastics on Distribution of Trace Heavy Metals in Seawater
NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kindai University
Host in iJURC SOHRIN, Yoshiki

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

A Spectroscopic Analysis on Bio-Degradation Processes of Polymer Thin Film Surfaces
AOKI, Takashi, Faculty of Fiber Science and Engineering, Kyoto Institute of Technology
Host in iJURC HASEGAWA, Takeshi

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

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY iJURC)

Crystal Structure Analysis of GraE from Root-Nodule-Forming Bacterium
OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University
Host in iJURC FUJII, Tomomi

Enhanced Production of Fast Ions by TNSA with Pre-Pulse Laser
SUNAHARA, Atsushi, Institute of Laser Engineering, Osaka University
Host in iJURC INOUE, Syunsuke

Development and Device Evaluation of New D- π -A Emitters Based on Fluorinated Triarylborone Acceptors
MARDER, Todd B., Julius-Maximilians-Universität Würzburg, Institut für Anorganische Chemie
Host in iJURC KAJI, Hironori 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

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

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

Study on the Physical Mechanism on Novel-Ternary Nanoparticle Formation
TATETSU, Yasutomi, Meio University
Host in iJURC TERANISHI, Toshiharu

Development of Collaborative Reaction Fields Based on Dinuclearization of Mononuclear Complexes
YAMAGUCHI, Yoshitaka, Graduate School 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, Institute of Bioinformatics & Systems Biology, National Chiao Tung University
Host in iJURC AKUTSU, Tatsuya I

Developing Data-Driven Deep Learning Approaches for Accurate Identification of Protease-Specific Substrate Targets and Cleavage Sites
SONG, Jiangning, Biomedicine Discovery Institute, Monash University
Host in iJURC AKUTSU, Tatsuya I

Unveiling the Genomic Contents of Ecologically Important Marine Giant Viruses
DELMONT, Tom, CNRS, Genoscope, UMR8030
Host in iJURC OGATA, Hiroyuki I

Revealing Associations between Giant Viruses and Eukaryotes in the Global Ocean through Community Networks Inference and Mining
CHAFFRON, Samuel, LS2N, CNRS UMR6004
Host in iJURC ENDO, Hisashi I

Comprehensive Analysis of Viral Succession during the Transition of Multiple Types of Algal Blooms
NAGASAKI, Keizo, Faculty of Agriculture and Marine Science, Graduate School of Integrated Arts and Sciences, Kochi University
Host in iJURC OGATA, Hiroyuki

Effective Molecular Network Analysis and Application to Medical and Agricultural Research
KAYANO, Mitsunori, Research Center for Global Agromedicine, Obihiro University of Agriculture and Veterinary Medicine
Host in iJURC MAMITSUKA, Hiroshi

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

Exploration of Cycloaddition Properties of Guanidine Functionalized Isobenzofurans
MARGETIC, Davor, Division of Organic Chemistry and Biochemistry, Laboratory for Physical Organic Chemistry, Rudjer Boskovic Institute
Host in iJURC MURATA, Yasujiro

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

Development of Thermally Activated Delayed Fluorescent Materials Based on Through-Space Charge Transfer Using Dibenzophenazine as an Electron-Acceptor
TAKEDA, Youhei, Department of Applied Chemistry, Graduate School of Engineering, Osaka University
Host in iJURC KAJI, Hironori

Development of Nonsymmetrical Organic Semiconducting Molecules Toward Efficient Photovoltaics
SUZUKI, Mitsuharu, Graduate School of Engineering, Osaka University
Host in iJURC MURATA, Yasujiro

Synthesis and Properties of π -Conjugated Zwitterions with Negligible Solvatochromism
SHIMIZU, Akihiro, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University
Host in iJURC HIROSE, Takashi

Host-Guest Complexation of Cyclohexa-2,7-Anthrylene Ethynylene Derivatives with [n]CPP
KOBAYASHI, Kenji, Research Institute of Green Science and Technology, Shizuoka University
Host in iJURC YAMAGO, Shigeru

Trace Metal Elemental and Isotopic Composition in the North Pacific Ocean: Sources and Internal Cycling (2)
HO, Tung-Yuan, Research Center for Environmental Changes, Academia Sinica
Host in iJURC SOHRIN, Yoshiki

Resolving the Structure-Dynamics-Property Relationship in Polymer Nanocomposites under Uniaxial Stretching
KOGA, Tadanori, Department of Material Science and Chemical Engineering, Stony Brook University
Host in iJURC TAKENAKA, Mikihiro

High Frequency Response of Polymeric Liquids: Rheology and Dielectric Relaxation
SUKUMARAN, Sathish K., Graduate School of Organic Materials Science, Yamagata University
Host in iJURC SATO, Takeshi

Vibronic Effect between Photon and Energy Conversions Studied by Solid State NMR and Time Resolved EPR Spectroscopy
KOBORI, Yasuhiro, Laser Molecular Photoscience Laboratory, Molecular Photoscience Research Center, Kobe University
Host in iJURC KAJI, Hironori

Spatial Distribution of Nanostructures Composed of Sulfur Element in Polymer Thin Films
FUJIWARA, Akihiko, School of Engineering, Kwansei Gakuin University
Host in iJURC TAKENAKA, Mikihiro

Structure Analysis of Polymer Materials Having Sulfur Atoms in a Wet State by Resonant Small-Angle Scattering Methods
YAMAMOTO, Katsuhiro, Department of Life Science & Applied Chemistry, Graduate School of Engineering, Nagoya Institute of Technology
Host in iJURC TAKENAKA, Mikihiro

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

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

Glass Transition and Molecular Dynamics of Guest Low Mass Molecules in the Clathrate of Polymer Crystals
URAKAWA, Osamu, Department of Macromolecular Science, Osaka University
Host in iJURC MATSUMIYA, Yumi

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

Nonlinear Rheological Behavior of Telechelic Ionomer with a Distribution of Number of Ionic Stickers at the Ends
ZHANG, Zhijie, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences (CAS)
Host in iJURC MATSUMIYA, Yumi

Role of PX-PH-Type Phospholipase Ds in Plant Intracellular Membrane Traffic
OHASHI, Yohei, MRC Laboratory of Molecular Biology, University of Cambridge
Host in iJURC AOYAMA, Takashi

Self-Assembling Adjuvant-Built-In Vaccines for Cancer Immune Therapy
LI, Yan-Mei, Department of Chemistry, Tsinghua University
Host in iJURC UESUGI, Motonari

Application of Ferrimagnets for Spintronics Devices
SAMARDAK, Alexander, School of Natural Science, Far Eastern Federal University
Host in iJURC ONO, Teruo

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

Optimizing Sampling Devices and Procedures to Quantify Sources of Metals and Microplastics in Metro Manila, Philippines' Water Resources

CID-ANDRES, Abigail P., Department of Physical Sciences, College of Science, Polytechnic University of the Philippines,

Host in iJURC SOHRIN, Yoshiki I F

Verification and Development of Dynamic Stiction Theory
NAKANO, Ken, Faculty of Environment and Information Sciences, Yokohama National University

Host in iJURC TSUJII, Yoshinobu I

Novel Strategy for Intracellular Delivery of Nanomedicines
PUJALS, Sílvia, Nanoscopy for Nanomedicine Group, Institute for Bioengineering of Catalonia (IBEC)

Host in iJURC FUTAKI, Shiroh I F

Analysis of Novel Transporters for Strigolactones or Their Biosynthetic Intermediates

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

Host in iJURC MASHIGUCHI, Kiyoshi I

1,3-Dipolar Cycloaddition Reactions of Cycloparaphenylenes with Azomethine Ylide

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

Host in iJURC YAMAGO, Shigeru I

Investigation of Relationship between Molecular Structure and Viscoelastic Parameters of Model Poly(Alkylstyrene)s.

TAKANO, Atsushi, Nagoya University

Host in iJURC MATSUMIYA, Yumi

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

Demonstration of Topological Phase Control in Chalcogenide Superlattices

MOROTA, Misako, Device Technology Research Institute, National Institute of Advanced Industrial Science and Technology(AIST)

Host in iJURC ONO, Teruo F

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

Analysis of Membrane Lipid-Dependent Fermentation Stress Response in Acetic Acid Bacteria

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

Host in iJURC KURIHARA, Tatsuo

Thermal Conduction of Pseudo-Ordered Oxide Glasses
MASUNO, Atsunobu, Graduate School of Science and Technology, Hirotsaki University

Host in iJURC SHIMAKAWA, Yuichi

Development of Eu Separation Method by Solid Phase Extraction Using Surfactant

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

Host in iJURC SOHRIN, Yoshiki

Study on Water Freezing with Lignocellulose Nanofibers and Their Surface Modification Toward Functional Materials

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

Host in iJURC TSUJII, Yoshinobu

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

HATANO, Osamu, School of Medicine, Nara Medical University

Host in iJURC NAKAMURA, Masaharu

Switching of Aromaticity/Anti-Aromaticity of Oxidized Cycloparaphenylenes

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

Host in iJURC YAMAGO, Shigeru

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, Syunsuke

EXPANDING SUBJECTS

(ON-DEMAND FROM RELATED COMMUNITIES)

Role of Phosphoinositide Signaling in Pollen Development

ZHONG, Sheng, School of Life Sciences, Peking University

Host in iJURC AOYAMA, Takashi I F

Site-Selective Protein Acetylation by a Small Molecule

ZHOU, Lu, School of Pharmacy, Fudan University

Host in iJURC UESUGI, Motonari I

Orbitronics with New Material Systems

KIM, Sanghoon, University of Ulsan

Host in iJURC ONO, Teruo I

Study of Characteristics of Spin Wave in Magnetic Insulator

KIM, Kab-Jin, Department of Physics, Korea Advanced Institute of Science and Technology

Host in iJURC ONO, Teruo I

Highly Efficient Red Thermally Activated Delayed Fluorescence Emitters with Sterically Hindered Donor Skeleton

KWON, Jang Hyuk, Department of Information Display

Host in iJURC KAJI, Hironori 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

- 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
- Fabrication of Nanotopographical Polymer Surfaces for Bactericidal Properties-III
 ENDOH, 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
- Development of Semiconductor Quantum Dot Solid Films and Their Charge Carrier Dynamics
 TACHIBANA, Yasuhiro, School of Engineering, RMIT University
Host in iJURC TERANISHI, Toshiharu 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
- 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
- Research Toward Stable NV Centers at Shallow Region and Spin Dynamics in Diamond
 BALASUBRAMANIAN, Gopalakrishnan, Leibniz institute for surface engineering, Leipzig, Germany
Host in iJURC MIZUOCHI, Norikazu I
- Research of Quantum Controls in Multi-Qubit Diamond Quantum Processors and Quantum Sensors
 DOHERTY, Marcus W., Research School of Physics and Engineering, Australian National University
Host in iJURC MIZUOCHI, Norikazu I
- Molecular Mechanisms for the Inactivation of a Growth Hormone in Rice
 HE, Zuhua, Chinese Academy of Sciences, CAS Center for Excellence in Molecular Plant Sciences, Institute of Plant Physiology and Ecology
Host in iJURC YAMAGUCHI, Shinjiro I
- Dendritic Amphiphilic Block Copolymers as Additive for Polyvinylidene fluoride Based Membranes
 SEMSARILAR, Mona, Institut Europeen des Membranes (IEM), CNRS
Host in iJURC YAMAGO, Shigeru I
- Search for Four-Wave-Mixing in the Vacuum-Unveiling Dark Components in the Universe –
 HOMMA, Kensuke, Physics, Hiroshima University
Host in iJURC INOUE, Syunsuke I
- Development of Perovskite and Perovskite-Like Emitters and Their Applications
 LIN, Hao-Wu, Department of Materials Science and Engineering, National Tsing Hua University, Taiwan
Host in iJURC WAKAMIYA, Atsushi I
- Immune-Stimulatory Nano-Assemblies
 YAMASAKI, Sho, Research Institute for Microbial Disease, Osaka University
Host in iJURC UESUGI, Motonari
- Self-Assembling Molecules for Improvement of Cardiomyocyte Engraftment
 SHIBA, Yuji, School of Medicine, Shinshu University
Host in iJURC UESUGI, Motonari
- Development of π -Conjugated Polymers for High-Efficiency Non-Fullerene Solar Cells
 OSAKA, Itaru, Department of Applied Chemistry, Graduate School of Engineering and Applied Chemistry Program, Graduate School of Advanced Science and Engineering, Hiroshima University
Host in iJURC WAKIOKA, Masayuki
- Study of Spin Dynamics in Garnet Nanocrystal 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
- Electronic and Spintronic Properties of Multilayer System Including NiCo_2O_4 and Fe_3O_4
 NAGAHAMA, Taro, Solid State Chemistry Laboratory, Faculty of Engineering, Hokkaido University
Host in iJURC ONO, Teruo
- Development of Thermally Activated Delayed Fluorescence Materials with Nanosecondorder Reverse Intersystem Crossing
 AIZAWA, Naoya, RIKEN Center for Emergent Matter Science
Host in iJURC KAJI, Hironori
- Mechanism of the RISC in TADF Studied by Time-Resolved Laser Spectroscopy
 YAMAKATA, Akira, Graduate School of Engineering, Toyota Technological Institute
Host in iJURC KAJI, Hironori
- Functional Characterization of Extracellular Vesicles Produced by Intestinal Bacteria and Development of Their Applications
 YAMASAKI, Shino, Department of Chemistry and Materials Engineering, Kansai University
Host in iJURC KURIHARA, Tatsuo F
- Synthesis and Study of Oxides with Unusually High-Valent Cation
 SAITO, Takashi, High Energy Accelerator Research Organization (KEK)
Host in iJURC SHIMAKAWA, Yuichi
- Fine Synthesis of Polymer Brush on Nano-Platelet for Functional Photonic LC
 UCHIDA, Yoshiaki, Graduate School of Engineering Science, Osaka University
Host in iJURC OHNO, Kohji
- Water in the Polymer Brush Layer: Structure and Freezing Behavior
 GENMEI, Makoto, Graduate School of Innovative Life Science, Toyama University
Host in iJURC OHNO, Kohji

Giant Magnetic Resistance on Single-Electron Transistor
MAJIMA, Yutaka, Laboratory for Materials and Structures,
Tokyo Institute of Technology
Host in iJURC TERANISHI, Toshiharu

Identification of Novel Cellular Uptake Stimulation Proteins
KUWATA, Keiko, Institute of Transformative Bio-Molecules,
Nagoya University
Host in iJURC FUTAKI, Shiroh [F]

Cellular Uptake Using Macropinocytosis
MAEKAWA, Masashi, Keio University
Host in iJURC FUTAKI, Shiroh

Research by Atomically Flat Surface Diamond for Quantum
Information Science and Technology
TOKUDA, Norio, Institute of Science and Engineering, Faculty
of Electrical and Computer Engineering, Kanazawa University
Host in iJURC MIZUOCHI, Norikazu

Development of Quantum Technology and Diamond Synthesis
for Higher Sensitivity of NV Quantum Sensor
MAKINO, Toshiharu, National Institute of Advanced Industrial
Science and Technology Power Industrial Technology Research
Institute
Host in iJURC MIZUOCHI, Norikazu

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

Coupling of Concentration Fluctuation and Orientation Fluctuation
in Mixture of Nematic Liquid Crystal and Solvent
SHIMADA, Ryoko, Japan Women's University
Host in iJURC WATANABE, Hiroshi [F]

SUBJECTS FOCUSING OF JOINT USAGE OF iJURC/ ICR FACILITIES

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

Tackling the Electronic Instability of Charge-Density Waves by
Electron Energy-Loss Spectroscopy Use
CHU, Ming-Wen, Center for Condensed Matter Sciences, Na-
tional Taiwan University
Host in iJURC KURATA, Hiroki [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]

Synthesis and Characterization of Novel Group 16 Element
Compounds
MINOURA, Mao, Department of Chemistry, College of Science,
Rikkyo University
Host in iJURC TOKITOH, Norihiro [I] [F]

Analyses of Organic Crystals and Thin Films Using Solid-State
NMR Spectroscopy
IE, Yutaka, Department of Soft Nanomaterials Nanoscience and
Nanotechnology Center, Osaka University
Host in iJURC KAJI, Hironori

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

Radiative Lifetime Control of Rare-Earth Codoped Nanoparticles
SAITO, Hikaru, Institute for Materials Chemistry and Engineer-
ing, Kyushu University
Host in iJURC KURATA, Hiroki

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 Engi-
neering, College of Engineering, Ibaraki University
Host in iJURC TOKITOH, Norihiro

Synthesis and Structural Characterization of Halostannylenes
MATSUO, Tsukasa, Faculty of Science and Engineering, Kindai
University
Host in iJURC TOKITOH, Norihiro

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]

Synthesis and Structures of Cationic Aromatics Bearing Thiopy-
rylium 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, Department of Chemistry and Material Technology,
Kyoto Institute of Technology
Host in iJURC NAKAMURA, Masaharu

SUBJECTS ENCOURAGING JOINT PROGRAM

Determine the Three-Dimensional Structure of ^{13}C 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]

Modulation of In-Cell Protein-Protein Interactions Using Mid-
Sized Peptides ICR Partner
HAYASHI, Yoshio, The School of Pharmacy, Tokyo University
of Pharmacy and Life Sciences (TUPLS)
Host in iJURC FUTAKI, Shiroh [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 2021)

Double-Holed Fullerenes

Hashikawa, Y.; Fushino, T.; Murata, Y., *J. Am. Chem. Soc.*, **142**, 20572-20576 (2020).

Abstract

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. Herein, we report 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.

Observation of Superconducting Diode Effect

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

Abstract

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 $[Nb/V/Ta]_n$ 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 $[Nb/V/Ta]_n$ 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.

Discovery of Self-Assembling Small Molecules as Vaccine Adjuvants

Jin, S.; Vu, H. T.; 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., *Angew. Chem. Int. Ed.*, **60**(2), 961-969 (2021).

Abstract

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.

Highly Luminescent $CsPbBr_3@Cs_4PbBr_6$ Nanocrystals and Their Application in Electroluminescent Emitters

Bao, Z.; Chiu, H.-D.; Wang, W.; Su, Q.; Yamada, T.; Chang, Y.-C.; Chen, S.; Kanemitsu, Y.; Chung, R.-J.; Liu, R.-S., *J. Phys. Chem. Lett.*, **11**, 10196-10202 (2020).

Abstract

Zero-dimensional perovskite nanocrystals (NCs) are becoming the most attractive material due to their excellent optical performance and better stability compared with high-dimensional perovskite. However, their application in electroluminescent (EL) emitters for high-quality displays is still limited. In this work, we successfully achieved $CsPbBr_3@Cs_4PbBr_6$ NCs around 13.9 ± 0.2 nm by using the hot-injection method. Additional $SnBr_2$ was mixed in the $PbBr_2$ precursor to provide extra Br^- ions and reduce the excessive amount of Pb^{2+} ions to promote the formation of $CsPbBr_3@Cs_4PbBr_6$. Time resolution photoluminescence analysis indicated that the green emission of our $CsPbBr_3@Cs_4PbBr_6$ NCs originated from the embedded $CsPbBr_3$ NCs, which corresponds to our previous research. The Cs_4PbBr_6 crystals passivated the surface of $CsPbBr_3$ NCs, resulting in the absence of trions for the high photoluminescence quantum yield. The as-synthesized $CsPbBr_3@Cs_4PbBr_6$ NCs were used to fabricate quantum dot light-emitting diode (QLED) devices with the highest current efficiency of 4.89 cd/A. This is the best performance of the $CsPbBr_3@Cs_4PbBr_6$ -system QLED device, which reveals the great potential of $CsPbBr_3@Cs_4PbBr_6$ NCs and will inspire further study of zero-dimensional perovskite composite NCs for EL emitters.

Biogeography of Marine Giant Viruses Reveals Their Interplay with Eukaryotes and Ecological Functions

Endo, H.; Blanc-Mathieu, R.; Li, Y.; Salazar, G.; Henry, N.; Labadie, K.; de Vargis, C.; Sullivan, M. B.; Bowler, C.; Wincker, P.; Karp-Boss, L.; Sunagawa, S.; Ogata, H., *Nat. Ecol. Evol.*, **4**, 1639-1649 (2020).

Abstract

Nucleocytoplasmic large DNA viruses (NCLDVs) are ubiquitous in marine environments and infect diverse eukaryotes. However, little is known about their biogeography and ecology in the ocean. By leveraging the *Tara* Oceans pole-to-pole metagenomic data set, we investigated the distribution of NCLDVs across size fractions, depths and biomes, as well as their associations with eukaryotic communities. Our analyses reveal a heterogeneous distribution of NCLDVs across oceans, and a higher proportion of unique NCLDVs in the polar biomes. The community structures of NCLDV families correlate with specific eukaryotic lineages, including many photosynthetic groups. NCLDV communities are generally distinct between surface and mesopelagic zones, but at some locations they exhibit a high similarity between the two depths. This vertical similarity correlates to surface phytoplankton biomass but not to physical mixing processes, which suggests a potential role of vertical transport in structuring mesopelagic NCLDV communities. These results underscore the importance of the interactions between NCLDVs and eukaryotes in biogeochemical processes in the ocean.



VISITING PROFESSORS'
ACTIVITIES IN ICR



Vis Prof
NAKAJIMA, Atsushi
(D Sc)

Laboratory of Organoelement Chemistry
Professor, Department of Chemistry, Faculty of Science and Technology, Keio University (3-14-1 Hiyoshi Kohoku-ku, Yokohama 223-8522)

Lecture at ICR
Creation and Characterization of Silicon-Cage Nanoclusters



Vis Prof
SODEOKA, Mikiko
(D Pharm)

Laboratory of Chemical Biology
Chief Scientist, RIKEN (2-1, Hirosawa, Wako, Saitama 351-0198)

Lecture at ICR
Affinity Labeling for Analyzing Protein-Protein Interaction



Vis Prof
INOUE, Tadashi
(D Eng)

Laboratory of Molecular Rheology
Professor, Department of Macromolecular Science, Graduate school of Science, Osaka University (1-1 Machikaneyama-cho, Toyonaka, Osaka 560-0043)

Lecture at ICR
On the Relationship between Viscoelasticity and Chain Rigidity of Polymers



Vis Prof
YABUUCHI, Naoaki
(D Eng)

Laboratory of Advanced Solid State Chemistry
Professor, Department of Chemistry and Life Science, Yokohama National University (79-5 Tokiwadai, Hodogaya-ku, Yokohama, Kanagawa 240-8501)

Lecture at ICR
Design and Development of New Oxide Battery Materials



Vis Assoc Prof
KISHI, Ryohei
(D Sc)

Laboratory of Polymer Controlled Synthesis
Associate Professor, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University (1-3 Machikaneyama, Toyonaka, Osaka 560-8531)

Lecture at ICR
1. Chemical Bond Theory Based on Molecular Orbital and Valence Bond Methods: From Hydrogen Molecules to Open-Shell Singlet Molecules
2. Structure-Property Relationships and Molecular Design of Open-Shell Singlet Molecular Systems: Interplay of Theory-Calculation-Synthesis-Measurement



Vis Assoc Prof
KONDO, Yoshiko
(D Agr)

Laboratory of Hydrospheric Environment Analytical Chemistry

Associate Professor, Graduate School of Fisheries and Environmental Sciences, Nagasaki University (1-14 Bunkyo-machi, Nagasaki 852-8521)

Lecture at ICR
Dynamics of Trace Metals such as Fe in the Ocean



Vis Assoc Prof
KODAIRA, Satoshi
(D Sc)

Laboratory of Particle Beam Science
Group Leader, Radiation measurement group, Department of Radiation Measurement and Dose Assessment, National Institute of Radiological Sciences, National Institutes for Quantum Science and Technology (4-9-1 Anagawa, Inage, Chiba 263-8555)

Lecture at ICR
Verification of Radiochemical Reaction Mechanism for FLASH Radiotherapy with Electron Beams



Vis Assoc Prof
ISHIDA, Takashi
(D Agr)

Laboratory of Chemical Life Science
Associate Professor, School of Computing, Tokyo Institute of Technology (2-12-1 Ookayama, Meguro-ku, Tokyo 152-8550)

Lecture at ICR
Deep Learning for Prediction and Analysis of Protein Structures



Prof Em KANEHISA, Minoru (D Sc)
Appointed as Res (pt) at ICR,
1 April 2012–31 March 2022



PERSONAL

Retirement

Professor TOKITOH, Norihiro
Division of Synthetic Chemistry
– Organoelement Chemistry –



On March 31st 2022, Dr. Norihiro Tokitoh retired from Kyoto University after 22 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Tokitoh was born in Miyazaki Prefecture on January 26, 1957. He graduated from Faculty of Science, the University of Tokyo in 1979, and entered the graduate school. He received the doctoral degree under the guidance of Professor Naoki Inamoto in 1985. He was appointed to a research associate at International Christian University in 1985 and to an assistant professor at Tsukuba University in 1986. In 1989, he was appointed to an assistant professor at the University of Tokyo, and promoted as an associate professor in 1994. In 1998, he moved to Kyushu University as a professor at Institute for Fundamental Research of Organic Chemistry. In 2000, he was employed as a professor at ICR, Kyoto University and has been working until 2022. During this time, he served as a guest professor at Institute for Molecular Science (2001–2003) and as a visiting professor at Technische Universität Braunschweig (2004–2007) and at Universität Bonn (2012–2014) in Germany.

Throughout his academic career, Dr. Tokitoh's research has been focused on "main group element chemistry", especially on novel bonding and structures of highly reactive species including "heavy elements", that is, main group elements in the periods 3rd through 6th. He is one of the pioneers in the chemistry of multiply bonded and low-coordinated compounds containing heavy main group elements and has created a number of novel compounds with many unique structures and properties by taking advantage of a kinetic stabilization method utilizing original steric protection groups developed by himself. It is noteworthy that he has made significant impacts on the research field by synthesizing and isolating novel compounds including elements of various groups and periods without limiting the elements to be studied. He systematically studied their structures and properties and verified the differences and similarities in the properties of elements. Furthermore, based on his pioneering research achievements, he has expanded his research into the construction of extended π -electron systems, transition metal complexes, and small molecule activation, opening new areas including new reactions. These achievements have been published as 468 original papers and 25 reviews in academic journals and 24 books (edited and co-authored).

His educational contribution to Kyoto University is also noteworthy. He has supervised 71 graduate students (45 Ph. D. degrees and 49 Master degrees) as a professor at Department of Chemistry, Graduate School of Science, and sent them out to academia and industry.

He has served on the boards and committees of many chemistry-related academic societies, including as President of the Society of Silicon Chemistry, Japan (2016–2018) and President of the Society of Physical Organic Chemistry, Japan (2018–2022). He has also served

as an editorial board member and editor-in-chief of many domestic and international journals, including the Bulletin of the Chemical Society of Japan (2013–2016), and as a member of the international advisory board of various international conferences representing Japan, greatly contributing to the development of the field of chemistry. He has also organized two international conferences held at ICR (the 10th International Conference on Heteroatom Chemistry in 2012 and the 15th International Symposium on Inorganic Ring Systems in 2018, the latter of which was first held in Japan), and is highly trusted by researchers in Japan and abroad. In addition, he has given an extremely large number (73) of plenary, keynote, and invited lectures at a variety of international conferences, reflecting the results of his continuous world-leading research.

His contribution to the administration of Kyoto University and ICR is also very significant. At ICR, he served as Deputy Director (2005–2008) and as Director (2008–2012 and 2014–2018; totally 7 and half years). In addition, he served as Director, Kyoto Univ. Pioneering Research Unit for Next Generation (2006–2008), Dean, Kyoto University, Division of Natural Sciences (2016–2018), Director, Kyoto University, Section of Integrated Chemistry (2016–2018), Vice-Director, Kyoto University, Institute for Liberal Arts and Sciences (2017–2020), and Director, Kyoto University, Research Coordination Alliance (2018–2020). Since 2020, he is serving as Executive Vice-President of Kyoto University for Research, Evaluation, and Industry-Government-Academia Collaboration.

For his achievements, he was awarded Special Lectureship Award for Young Generation from the Chemical Society of Japan in 1991, Incentive Award from the Society of Synthetic Organic Chemistry, Japan in 1992, Incentive Award from the Society of Silicon Chemistry, Japan in 1992, Japan IBM Science Award in 1998, Chemical Society of Japan Award for Creative Work in 2003, Alexander von Humboldt Research Award in 2003/Re-invitation in 2013, Lectureship Award of National Science Council, Taiwan in 2007, the 3rd Kim Yong Hae Lectureship Award KAIST, Korea in 2010, Best Reviewer Commendation from Japan Society for the Promotion of Science in 2010 and 2017, JSBBA Award from the Japan Society for Bioscience, Biotechnology, and Agrochemistry in 2017, and Society Award from the Society of Silicon Chemistry, Japan in 2019. In addition, it is noteworthy that he received BCSJ Award from the Chemical Society of Japan seven times (2002, 2005, 2007, 2009, 2010, 2013 and 2016), making him the most frequent recipient of this award.

Dr. Tokitoh'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.

Retirement

Professor WATANABE, Hiroshi
Division of Multidisciplinary Chemistry
– Molecular Rheology –



On March 31, 2022, Dr. Hiroshi Watanabe retired from Kyoto University and was honored with the title of Professor Emeritus. He was born in Kagawa Prefecture on January 30, 1957. In 1979, he graduated from Faculty of Science, Osaka University, and entered the graduate school with a guidance of Prof. Tadao Kotaka. He quitted the graduate school in 1983 to start working as Research Associate in Prof. Kotaka's lab, received a doctoral degree from Osaka University in 1985, and was promoted to Assistant Professor in 1987. In 1987–1989, he made a research stay at Department of Chemical Engineering and Materials Science, University of Minnesota, as Post-Doc working with Prof. Matthew Tirrell (while keeping the Assistant Professor position in Osaka University). He moved to Prof. Kunihiro Osaki's lab at the Institute for Chemical Research (ICR), Kyoto University, as Associate Professor in 1994, and was promoted to Professor in 2003.

Dr. Watanabe has been investigating dynamics and rheology of various softmatters. He combined several experimental methods, for example, rheological, dielectric, and small angle x-ray and neutron scattering (SAXS and SANS) methods, with theoretical model analyses to reveal physical factors governing the dynamic behavior of softmatters, as explained below for some examples.

AB-type diblock copolymers with relatively short B blocks form spherical micelles in A-selective solvents, with the unsolvated B blocks forming micellar cores and the solvated A blocks serving as corona chains. He combined rheological and SAXS methods to find that those systems exhibit plasticity because of a regular lattice of the micelles stabilized by an osmotic interaction between the corona chains. From rheo-SANS experiments, he revealed that the plastic flow occurs at boundaries between grains of the micellar lattice without disruption of the lattice itself and that the force sustained by the lattice is consistent with a magnitude of the osmotic interaction. He also demonstrated that the micelles are randomly dispersed to lose their plasticity in A-homopolymers (polymeric solvents) that screen the osmotic interaction, thereby confirming the origin of the plasticity explained above.

Those micellar dispersions exhibit polymeric characters in short time scales but behave similarly to suspensions of Brownian particles in long time scales. For investigation of this similarity, he conducted rheo-SANS experiments for suspensions of nano-silica particles. He found that the viscosity η of the suspensions first decreases and then increases on an increase of the flow rate, with the decrease of η reflecting just a weak decrease of the placement entropy of the particles under slow flow whereas the increase of η resulting from jamming of the particles under flow faster than their Brownian motion. He re-

vealed that the diblock micellar dispersions exhibit the decrease of η with the same mechanism related to the placement entropy of the micelles but no increase of η because the micellar corona chains behave as polymer brushes and prevent the micellar cores from the jamming.

He also found that the short time behavior of the micellar dispersions is governed by the entanglement among the corona chains, as characteristic to polymers. This finding led him to study a detailed molecular aspect of entanglement for model systems, blends of chemically identical long and short homopolymers. His experiments identified, for the first time in the world, full viscoelastic relaxation of dilute long chains activated by the short chain motion, known as constraint release (CR) relaxation. Furthermore, for polymers having electrical dipoles parallel along the chain backbone, he realized that the viscoelastic and dielectric relaxation functions reflect the same chain dynamics but with different averaging moments, and formulated a theoretical relationship between those functions. He tested this relationship for viscoelastic and dielectric data of various blends to establish that a coarse-grained view of CR, known as dynamic tube dilation, is valid if a spatial scale of the CR-activated motion of the chain is properly incorporated in that view. He also realized the importance of the dynamics of short unentangled chains in the nonlinear behavior of long entangled chains under fast flow, and analyzed the unentangled chain dynamics by considering flow effects on the local friction and elasticity as well as on the Brownian force.

His achievements have been highly appreciated in the worldwide community of softmatter science, as evidenced from awards for him that include the Fellow of the American Physical Society (2005), the Research Award of the Society of Polymer Science, Japan (2008), the Research Award of the Society of Rheology, Japan (2012), and the Bingham Award of the Society of Rheology, USA (2015). Furthermore, he served to the community through various roles, for example, the President of the Society of Rheology, Japan (2015–2017), the President of the International Committee on Rheology (2016–2020), and the Associate Editor of *Macromolecules* issued by the American Chemical Society (2011-present).

In summary, Dr. Watanabe has contributed to ICR and Kyoto University through his scientific research and education as well as his role of Vice-Director of ICR (2008–2012). His open-minded scientific approach, based on the principle of rheology cast in the famous phrase “*πάντα ῥεῖ* (*everything flows, and changes with time*)”, will surely encourage further studies of softmatters.

Awards

OMATSU, Yamato



CSJ Student Presentation Award 2021

The 101st CSJ Annual Meeting (2021)

“Synthesis of Unsaturated Silicon Clusters Utilizing Asymmetrically Substituted Disilanes”

The Chemical Society of Japan

28 April 2021

HIROSE, Takashi



Outstanding Reviewer for Chemical Communications in 2020

“Outstanding Reviewer for Chemical Communications in 2020”

The Royal Society of Chemistry

26 May 2021

UEDA, Yoshihiro



Young Scientist's Research Award in Natural Product Chemistry

“Regio- and Stereodivergent Synthesis of Ellagitannins based on Sequential Site-Selective Functionalization”

Young Scientist's Society of Natural Product Chemistry

26 July 2021

LI, Zhanzhao



ICR Award for Graduate Students

“Determinants of Crystal Structure Transformation of Ionic Nanocrystals in Cation Exchange Reactions”

Institute for Chemical Research, Kyoto University

10 December 2021

TSUJII, Yoshinobu



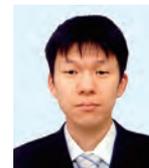
39th JSPM Award for Inovatory Development

“Development of Through-Pore Porous Particles and Their Application to Liquid Chromatography”

Japan Society of Powder and Powder Metallurgy

03 June 2021

SHIOTA, Yoichi



The Young Scientists' Award

The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology

“Research on Control of Magnetization Dynamics in Nanoscale Magnetic Multilayers”

Ministry of Education, Culture, Sports, Science and Technology

14 April 2021

FUTAKI, Shiroh



2020 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

27 January 2021

IWATA, Takahiro



ICR Award for Graduate Students

“Liquid Droplet Formation and Facile Cytosolic Translocation of IgG in the Presence of Attenuated Cationic Amphiphilic Lytic Peptides”

Institute for Chemical Research, Kyoto University

10 December 2021

SOHRIN, Yoshiki



The Geochemical Society of Japan Award 2021

“Geochemical Study on Trace Metals in the Hydrosphere Based on Stoichiometry and Stable Isotope Ratio”

The Geochemical Society of Japan

09 September 2021

The Japan Society for Analytical Chemistry Award, 2021

“Development of Precise Analytical Methods of Trace Metals and Their Isotopes for Innovation in Hydrosphere Environmental Chemistry”

The Japan Society for Analytical Chemistry

23 September 2021

TSUDZUKI, Taiku



Best Oral Presentation Award

67th Annual Meeting of the Japanese Biochemical Society, Kinki Branch

“Functions of the Surface Sugar Chain-Synthesizing Enzyme in Transport of a Cargo Protein in the Hypervesiculating Bacterium”

The Japanese Biochemical Society, Kinki Branch

29 May 2021

INOUE, Hiromu



Presentation Award

The 22nd Annual Meeting of Japanese Society for Extremophiles
“Screening of Genes Related to Extracellular Membrane Vesicle Production of *Shewanella vesiculosa* HM13 Using a Curvature-Sensing Peptide”

The Japanese Society for Extremophiles

20 November 2021

WAKAMIYA, Atsushi



The Chemical Society of Japan Award for Creative Work for 2020

“Study of Metal Halide Perovskite Solar Cells Based on Molecular Design and Highly Purified Precursor Materials”

The Chemical Society of Japan (CSJ)

20 March 2021

WAKAMIYA, Atsushi KANEMITSU, Yoshihiko

The 53th Ichimura Prize in Science against Global Warming for Distinguished Achievement

“Development of Efficient Film Type Solar Cells Using Printable Perovskite Semiconductors”

Ichimura Foundation for New Technology

19 April 2021



TRUONG, Minh Anh



Innovative PV Encouragement Award

18th "Next Generation Photovoltaic Power Generation System" Symposium (1st Japan Society for Photovoltaic Power Generation Academic Lecture)

"Development of Multipodal Hole Collecting Materials for Efficient Perovskite Solar Cells"

The Japan Photovoltaic Society (JSES)

16 November 2021

HU, Shuaifeng



Innovative PV Encouragement Award

18th "Next Generation Photovoltaic Power Generation System" Symposium (1st Japan Society for Photovoltaic Power Generation Academic Lecture)

"Interface Modification Strategies Using Surfactants for 23.6% Efficient Tin-Lead Perovskite Solar Cells"

The Japan Photovoltaic Society (JSES)

16 November 2021

KOSUGI, Yoshihisa



CSJ Student Presentation Award 2021

The 101st Annual Meeting of the Chemical Society of Japan
"Large Latent Heat and Barocaloric Effects at Charge Transfer Transitions of A-Site Ordered Perovskite Oxides"

The Chemical Society of Japan

19 March 2021

ICR Award for Graduate Students

"Clossal Barocaloric Effect by Large Latent Heat Produced by First-Order Intersite-Charge-Transfer Transition"

Institute for Chemical Research, Kyoto University

10 December 2021

IHOSHI, Makoto



Student Award for Outstanding Presentation

Spring Meeting of the Japan Society of Powder and Powder Metallurgy 2021

"Successive Phase Transition in A-Site Layer-Ordered Double-Perovskites RBaFe_2O_6 (R=Sm, Nd) with Unusually High Valence Fe Ions"

Japan Society of Powder and Powder Metallurgy

01 June 2021

TAHARA, Hirokazu



Kao Science Encouragement Award

"Quantum Coherent Coupling of Colloidal Nanocrystals Realized by Surface Ligand Control"

The Kao Foundation for Arts and Sciences

01 June 2021

Young Scientist Award of the Physical Society of Japan

"Quantum Coherent Dynamics of Photoexcited States in Semiconductor Nanostructures"

The Physical Society of Japan

14 March 2021

ENDO, Hisashi



ICR Award for Young Scientists

"Biogeography of Marine Giant Viruses Reveals Their Interplay with Eukaryotes and Ecological Functions"

Institute for Chemical Research, Kyoto University

10 December 2021

Paper Awards

MURATA, Yasujiro, *et al.*



BCSJ Award

Bulletin of the Chemical Society of Japan

“Mechanism of 2,6-Dichloro-4,4’-Bipyridine-Catalyzed
Diboration of Pyrazines Involving a Bipyridine-Stabilized
Boryl Radical”

The Chemical Society of Japan

05 June 2021

Poster Awards

HUANG, Guanglin



Poster Award

31st Symposium on Physical Organic Chemistry

“A Role of a Hydroxy Stopper: Kinetic and Thermodynamic Stabilization of H₂O₂ Encapsulated inside an Open-Cage C₆₀ Derivative”

The Society of Physical Organic Chemistry, Japan

23 September 2021

Obituary

Professor Emeritus
Dr. UEDA, Kunihiro (1940–2021)



Dr. Kunihiro Ueda, Professor Emeritus of Kyoto University, passed away on September 5, 2021, at the age of 81.

Dr. Ueda was born in Kyoto on 25th of May, 1940. He graduated from Kyoto University Faculty of Medicine in 1965 and finished an internship at Kyoto University Hospital in 1966. He studied medical chemistry at the Graduate School of Medicine, Kyoto University, under the supervision of Professor O. Hayaishi, and was granted a doctoral degree in 1973. In 1971, he was appointed as an instructor of the Institute for Chemical Research, Kyoto University. On leave from Kyoto University from 1974 to 1976, he studied molecular biology under Professor A. Komberg at Stanford University, USA. In 1981, he was promoted to a Lecturer of Medical Chemistry and, in 1985, an Associate Professor of Clinical Science and Laboratory Medicine, Kyoto University. In 1994, he was appointed as a full Professor of the Institute for Chemical Research, Kyoto University, and directed the Laboratory of Molecular Clinical Chemistry. He gave lectures at the Graduate School of Medicine and supervised the dissertation works of graduate students.

During his academic carrier, Dr. Ueda made a number of notable findings regarding the regulatory mechanisms of life. In particular, the discovery of “the third nucleic acid”, i.e. poly(ADP-ribose), with Dr. Y. Nishizuka in 1966 opened a new era of protein modification by coenzyme, NAD, and led him to a life-long enthusiasm for research of this novel polymer. His years’ effort resulted in the discovery and characterization of three key enzymes, one synthetic and two degradative, in poly(ADP-ribose) metabolism, isolation of poly(ADP-ribosyl) histones from animal tissues, immunohistochemical demonstration of poly(ADP-ribose) in human cells, finding of roles of poly(ADP-ribose) in DNA repair, carcinogenesis and apoptosis, development of specific inhibitors of the synthetase, and discovery of the inhibitors’ protective effects against ischemic or oxidative lesions in the brain and heart. All these achievements

formed landmarks in the history of poly(ADP-ribose) research and made Dr. Ueda one of the leaders in this research field in the world.

After moving to a clinical laboratory, he also undertook investigation of molecular etiology of Alzheimer’s disease and improvement of gene diagnostic techniques. His early finding of an age-related change in expression of A β amyloid precursors among patients was a pioneering work in understanding the pathogenesis of Alzheimer’s disease. He later disclosed a possible link between overactivation of poly(ADP-ribose) synthesis and neuronal degeneration in this disease. His efforts in developing methods for clinical gene testing resulted in commercialized products, Ampdirect™ for polymerase chain reaction and a transcription-reverse transcription-concerted reaction device.

For these distinguished contributions to science and biotechnology, he was awarded the Young Researcher Promotion Prize from the Japanese Biochemical Society, the Prize of the Japan Society of Vitaminology and Nutrition, and the Shibata Susumu Medal from the Clinical Pathology Promotion Foundation.

He served in the three Ministries’ Joint Committee for Ethics Guidelines for Human Genome/Gene Analysis Research. He chaired the Committee for Regulation of Human Genome/ Gene Analysis Research in Kyoto University. He served as members of Directors of many academic societies in Japan and has kept the presidency in the Society for Gene Diagnosis and Therapy since 2001. Internationally, he organized the First Japan-Italy Bilateral Seminar on ADP-riboses and Nitric Oxide (1997, Kyoto) and the Second IFCC-Roche Conference on Human Genomics (2000, Kyoto). He is an International Editor of the *Annals of Clinical Biochemistry* and the *Journal of Enzyme Inhibition and Medicinal Chemistry*.

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



PUBLICATIONS

INTERNATIONAL
RESEARCH
COLLABORATIONS

SELECTED GRANTS

THESSES



PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Jin, S.; Vu, H. T.; Hioki, K.; Noda, N.; Yoshida, H.; Shimane, T.; Ishizuka, S.; Takashima, I.; Mizuhata, Y.; Beverly, Pe K.; 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. Engl.*, **60**, 961-969 (2021).

Iwai, K.; Mizuhata, Y.; Tokitoh, N., Alkali-Metal-Ion-Centered Sandwich Structures of 4-Bromophenyl[tris(pentafluorophenyl)] Borates and Their Synthetic Utility, *Organometallics*, **40**, 570-577 (2021).

Murai, T.; Lu, W.; Kuribayashi, T.; Morisaki, K.; Ueda, Y.; Hamada, S.; Kobayashi, Y.; Sasamori, T.; Tokitoh, N.; Kawabata, T.; Furuta, T., Conformational Control in Dirhodium (II) Paddlewheel Catalysts Supported by Chalcogen-Bonding Interactions for Stereoselective Intramolecular C-H Insertion Reactions, *ACS Catal.*, **11**, 595-607 (2021).

Omatsu, Y.; Mizuhata, Y.; Tokitoh, N., Easily Separable Cyclic Oligosilanes with *p*-Methoxyphenyl Groups and Their Stereoselective Functionalization, *Eur. J. Inorg. Chem.*, **2021**, 1005-1012 (2021).

Hyakutake, R.; Yoshimura, T.; Sasamori, T.; Tokitoh, N.; Morisaki, K.; Kawabata, T., Decisive Effects of *c-n* Axial Chirality of Intermediary Enolates on the Stereochemical Course of β -Lactam Formation from β -Branched α -Amino Acid Derivatives via Memory of Chirality, *Heterocycles*, **103(2)**, 995-1010 (2021).

Yanagisawa, T.; Mizuhata, Y.; Tokitoh, N., A Novel Reactivity of Phosphanylaluminum (>P-Al<): Reversible Addition of a Saturated Interelement Bond to Olefins, *Chem. Eur. J.*, **27**, 11273-11278 (2021).

Nagata, M.; Min, H.; Watanabe, E.; Fukumoto, H.; Mizuhata, Y.; Tokitoh, N.; Agou, T.; Yasuda, T., Fused-Nonacyclic Multi-Resonance Delayed Fluorescence Emitter Based on Ladder-Thiaborin Exhibiting Narrowband Sky-Blue Emission with Accelerated Reverse Intersystem Crossing, *Angew. Chem. Int. Ed. Engl.*, **60**, 20280-20285 (2021).

Garcia, J. A.; Yukimoto, M.; Mizuhata, Y.; Tokitoh, N., A Unique 1,4-Silyl Group Migration from Carbon to Carbon: Formation of Benzylic Silane in the Reaction of Sterically Hindered Benzylic Telluride with Alkylolithium, *J. Organomet. Chem.*, **956**, 122119 (2021).

Nagata, M.; Oshiro, T.; Mizuhata, Y.; Tokitoh, N.; Hosoya, T.; Yamada, S.; Konno, T.; Fukumoto, H.; Kubota, T.; Agou, T., Synthesis of Carbazole-Fused Azaborines via a Pd-Catalyzed C-H Activation-Cyclization Reaction, *Bull. Chem. Soc. Jpn.*, **94(1)**, 21-23, (2021).

— Structural Organic Chemistry —

Zhang, S.; Hashikawa, Y.; Murata, Y., Cage-Expansion of Fullerenes, *J. Am. Chem. Soc.*, **143**, 12450-12454 (2021).

Suárez, M.; Makowski, K.; Lemos, R.; Almagro, L.; Rodríguez, H.; Herranz, M. Á.; Molero, D.; Ortiz, O.; Maroto, E.; Albericio, F.; Murata, Y.; Martín, N., An Androsterone-H₂@C₆₀ hybrid: Synthesis, Properties and Molecular Docking Simulations with SARS-Cov-2, *ChemPlusChem*, **86**, 972-981 (2021).

Hashikawa, Y.; Kizaki, K.; Murata, Y., Pressure-Induced Annulative Orifice Closure of a Cage-Opened C₆₀ derivative, *Chem. Commun. (Camb)*, **57**, 5322-5325 (2021).

Hashikawa, Y.; Hasegawa, S.; Murata, Y., Photochemical Orifice Expansion of a Cage-Opened C₆₀ Derivative, *Org. Lett.*, **23**, 3854-3858 (2021).

Hashikawa, Y.; Li, H.; Murata, Y., Reactions of C₆₀ with Pyridazine and Phthalazine, *Chem. Eur. J.*, **27**, 7507-7511 (2021).

Horii, Y.; Suzuki, H.; Miyazaki, Y.; Nakano, M.; Hasegawa, S.; Hashikawa, Y.; Murata, Y., Dynamics and Magnetic Properties of NO Molecules Encapsulated in Open-Cage Fullerene Derivatives Evidenced by Low Temperature Heat Capacity, *Chem. Phys.*, **23**, 10251-10256 (2021).

Hashikawa, Y.; Li, J.; Okamoto, S.; Murata, Y., Reactions on a 1,2-Dicarbonyl Moiety of a Fullerene Skeleton, *Chem. Eur. J.*, **27**, 7235-7238 (2021).

Shugai, A.; Nagel, U.; Murata, Y.; Li, Y.; Mamone, S.; Krachmalnicoff, A.; Alom, S.; Whitby, R. J.; Levitt, M. H.; Rödöm, T., Infrared Spectroscopy of an Endohedral Water in Fullerene, *J. Chem. Phys.*, **154**, 124311 (2021).

Hashikawa, Y.; Okamoto, S.; Murata, Y., Nonclassical Abramov Products Formed on Orifices of Cage-Opened C₆₀ Derivatives, *Chem. Eur. J.*, **27**, 4864-4868 (2021).

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. Engl.*, **60**, 2866-2870 (2021).

Hashikawa, Y.; Murata, Y., Water-Mediated Thermal Rearrangement of a Cage-Opened C₆₀ Derivative, *ChemPlusChem*, **86**, 1559-1562 (2021).

Sakamaki, D.; Tanaka, S.; Tanaka, K.; Takino, M.; Gon, M.; Tanaka, K.; Hirose, T.; Hirobe, D.; Yamamoto, H. M.; Fujiwara, H., Double Heterohelicenes Composed of Benzo[b]- and Dibenzo[b,i]phenoxazine: A Comprehensive Comparison of Their Electronic and Chiroptical Properties, *J. Phys. Chem. Lett.*, **12**, 9283-9292 (2021).

Fukushima, T.; Tamaki, K.; Isobe, A.; Hirose, T.; Shimizu, N.; Takagi, H.; Haruki, R.; Adachi, S.-I.; Hollamby, M. J.; Yagai, S., Diarylethene-Powered Light-Induced Folding of Supramolecular Polymers, *J. Am. Chem. Soc.*, **143**, 5845-5854 (2021).

Kubo, H.; Hirose, T.; Shimizu, D.; Matsuda, K., Donor-Acceptor Type [5]Helicene Derivative with Strong Circularly Polarized Luminescence, *Chem. Lett.*, **50**, 804-807 (2021).

Kato, S.-I.; Kumagai, R.; Abe, T.; Higuchi, C.; Shiota, Y.; Yoshizawa, K.; Takahashi, N.; Yamamoto, K.; Hossain, M. Z.; Hayashi, K.; Hirose, T.; Nakamura, Y., Arylene-Hexaynylene and -Octaynylene Macrocycles: Extending the Polyyne Chains Drives Self-Association by Enhanced Dispersion Force, *Chem. Commun. (Camb)*, **57**, 576-579 (2021).

Kubo, H.; Hirose, T.; Nakashima, T.; Kawai, T.; Hasegawa, J.-Y.; Matsuda, K., Tuning Transition Electric and Magnetic Dipole Moments: [7]Helicenes Showing Intense Circularly Polarized Luminescence, *J. Phys. Chem. Lett.*, **12**, 686-695 (2021).

Shimizu, A.; Ishizaki, Y.; Horiuchi, S.; Hirose, T.; Matsuda, K.; Sato, H.; Yoshida, J.-I., HOMO-LUMO Energy-Gap Tuning of π -Conjugated Zwitterions Composed of Electron-Donating Anion and Electron-Accepting Cation, *J. Org. Chem.*, **86**, 770-781 (2021).

Ohmura, T.; Morimasa, Y.; Ichino, T.; Miyake, Y.; Murata, Y.; Suginome, M.; Tajima, K.; Taketsugu, T.; Maeda, S., Mechanism of 2,6-Dichloro-4,4'-Bipyridine-Catalyzed Diboration of Pyrazines Involving a Bipyridine-Stabilized Boryl Radical, *Bull. Chem. Soc. Jpn.*, **94**, 1894-1902 (2021).

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Du S.; Hashikawa Y.; Ito H.; Hashimoto K.; Murata Y.; Hirayama Y.; Hirakawa K., Inelastic Electron Transport and Ortho-Para Fluctuation of Water Molecule in H₂O@C₆₀ Single Molecule Transistors, *Nano Lett.*, **21**, 10346-10353 (2021).

Hashikawa Y.; Murata Y., Synthesis and Oligomerization of CpM(CO)₂, *ACS Omega*, **6**, 34137-34141 (2021).

Hashikawa, Y.; Sadai S.; Murata, Y., Amino-Functionalized Cage-Opened C₆₀ Derivatives, *Org. Lett.*, **23**, 9586-9590 (2021).

— Synthetic Organic Chemistry —

Imayoshi, A.; Lakshmi, B. V.; 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).

Chen, G.; Arai, K.; Morisaki, K.; Kawabata, T.; Ueda, Y., Dirhodium-Catalyzed Chemo- and Site-Selective C-H Amidation of *N, N*-Dialkylanilines, *Synlett*, **32**, 728-732 (2021).

Shibayama, H.; Ueda, Y.; Tanaka, T.; Kawabata, T., Seven-Step Stereodivergent Total Syntheses of Punicafolin and Macaranginin, *J. Am. Chem. Soc.*, **143**, 1428-1434 (2021).

Murai, T.; Lu, W.; Kuribayashi, T.; Morisaki, K.; Ueda, Y.; Hamada, S.; Kobayashi, Y.; Sasamori, T.; Tokitoh, N.; Kawabata, T.; Furuta, T., Conformational Control in Dirhodium(II) Paddlewheel Catalysts Supported by Chalcogen-Bonding Interactions for Stereoselective Intramolecular C-H Insertion Reactions, *ACS Catal.*, **11**, 595-607 (2021).

Xing, Y.; Nikaido, M.; Murai, T.; Hamada, S.; Kobayashi, Y.; Sasamori, T.; Kawabata, T.; Furuta, T., Concise Synthesis of an Amide-Functionalized [7]Helicene-Like Molecule via Intramolecular Amidation, *Heterocycles*, **103**, 544-553 (2021).

Hyakutake, R.; Yoshimura, T.; Sasamori, T.; Tokitoh, N.; Morisaki, K.; Kawabata, T., Decisive Effects of C-N Axial Chirality of Intermediary Enolates on the Stereochemical Course of β -Lactam Formation from β -Branched α -Amino Acid Derivatives via Memory of Chirality, *Heterocycles*, **103**, 995-1010 (2021).

Ueda, Y., Site-Selective Molecular Transformation: Acylation of Hydroxy Groups and C-H Amination, *Chem. Pharm. Bull. (Tokyo)*, **69**, 931-944 (2021).

Hamada, S.; Yano, K.; Kobayashi, Y.; Kawabata, T.; Furuta, T., Oxidation of Cyclic Benzylic Ethers by an Electronically Tuned Nitroxyl Radical, *Tetrahedron Lett.*, **83**, 153404 (2021).

— Advanced Inorganic Synthesis —

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

Zhang, J.; Sakai, H.; Suzuki, K.; Hasobe, T.; Tkachenko, N. V.; Chang, I.-Y.; Hyeon-Deuk, K.; Kaji, H.; Teranishi, T.; Sakamoto, M., Near-Unity Singlet Fission on a Quantum Dot Initiated by Resonant Energy Transfer, *J. Am. Chem. Soc.*, **143**, 17388-17394 (2021).

Cho, K.; Yamada, T.; Tahara, H.; Tadano, T.; Suzuura, H.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Luminescence Fine Structures in Single Lead Halide Perovskite Nanocrystals: Size Dependence of the Exciton-Phonon Coupling, *Nano Lett.*, **21**, 7206-7212 (2021).

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Saruyama, M.; Sato, R.; Teranishi, T., Transformations of Ionic Nanocrystals via Full and Partial Ion Exchange Reactions, *Acc. Chem. Res.*, **54**, 765-775 (2021).

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DIVISION OF MATERIALS CHEMISTRY — Chemistry of Polymer Materials —

Miyazaki, M.; Nakano, K.; Tadokoro, C.; Vlădescu, S.-C.; Reddyhoff, T.; Sasaki, S.; Tsujii, Y., Enhancing Durability of Concentrated Polymer Brushes Using Microgrooved Substrates, *Wear*, **482-483**, 203984 (2021).

Watanabe, S.; Kodama, E.; Tadokoro, C.; Sakakibara, K.; Nakano, K.; Sasaki, S.; Tsujii, Y., Durability Improvement of Concentrated Polymer Brushes by Multiscale Texturing, *Tribol. Lett.*, **69**, 99 (2021).

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— Bio-knowledge Engineering —

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Güvenç Paltun, B.; Mamitsuka, H.; Kaski, S., Improving Drug Response Prediction by Integrating Multiple Data sources: Matrix Factorization, Kernel and Network-Based Approaches, *Brief. Bioinform.*, **22**, 346-359 (2021).

Nguyen, D. A.; Nguyen, C. H.; Mamitsuka H., A Survey on Adverse Drug Reaction Studies: Data, Tasks and Machine Learning Methods, *Brief. Bioinform.*, **22**, 164-177 (2021).

Nguyen, D. A.; Ngo, V. L.; Nguyen, K. A.; Nguyen, C. H.; Than, K., Boosting Prior Knowledge in Streaming Variational Bayes, *Neurocomputing*, **424**, 143-159 (2021).

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Güvenç Paltun, B.; Kaski, S.; Mamitsuka, H., Machine Learning Approaches for Drug Combination Therapies, *Brief. Bioinform.*, **22**(6), bbab293 (2021).

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HAKUBI PROJECT

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

Injac, S. D. A.; Xu, Y.; Denis Romero, F.; Shimakawa, Y., Pauli-paramagnetic and Metallic Properties of High Pressure Polymorphs of BaRhO₃ Oxides Containing Rh₂O₉ Dimers, *Dalton Trans.*, **50**, 4673-4679 (2021).

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

Tahara, H.; Sakamoto, M.; Teranishi, T.; Kanemitsu, Y., Collective Enhancement of Quantum Coherence in Coupled Quantum Dot Films, *Phys. Rev. B*, **104**, L241405 (2021).

INTERNATIONAL RESEARCH COLLABORATIONS

[Australia]

Monash University, Biomedicine Discovery Institute

[China, P.R.]

Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, State Key Laboratory of Polymer Physics and Chemistry

Fudan University, School of Computer Science

Fudan University, School of Pharmacy

Fudan University, Shanghai Key Lab of Intelligent Information

The University of Hong Kong, Department of Mathematics

Xi'an Jiaotong University, School of Mathematics and Statistics

[Croatia]

Ruder Bošković Institute, Laboratory for Physical Organic Chemistry, Division of Organic Chemistry and Biochemistry

[Cuba]

Universidad de la Habana, Laboratorio de Síntesis Orgánica, Facultad de Química

[Estonia]

National Institute of Chemical Physics and Biophysics

[Finland]

Aalto University, Department of Computer Science

Tampere University, Chemistry and Advanced Materials Group, Faculty of Engineering and Natural Sciences

[France]

Centre National de la Recherche Scientifique

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

[Germany]

European Molecular Biology Laboratory

Max-Planck Institute for Structure and Dynamics of Matter

[Hungary]

Hungarian Academy of Sciences, Eötvös Loránd University

[India]

Indian Institute of Engineering Science and Technology

[Italy]

University of Campania "Luigi Vanvitelli", Department of Experimental Medicine

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

[Korea, R.]

Sungkyunkwan University, School of Chemical Engineering

[Lithuania]

Kaunas University of Technology, Department of Organic Chemistry

[Norway]

University of Bergen, Department of Biology

[Russia]

Far Eastern Federal University, Institute of High Technologies and Advanced Materials

[Singapore]

Nanyang Technological University, School of Physical and Mathematica Sciences

[Spain]

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

Universidad Complutense de Madrid, Departamento de Química Orgánica, Facultad de Ciencias Químicas

[Taiwan]

Academia Sinica, Research Center for Environmental Changes

National Taiwan University, Center for Condensed Matter Sciences

[Thailand]

Suranaree University of Technology, School of Chemistry

[U.K.]

Imperial College London, Department of Mechanical Engineering

Keele University, School of Chemical and Physical Sciences

Southampton University, School of Chemistry

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

[U.S.A.]

Columbia University, Department of Chemistry

Lawrence Berkeley National Laboratory, Molecular Biophysics and Integrated Bioimaging Division

Stanford University, Department of Chemistry, SLAC National Accelerator Laboratory

Stony Brook University, Department of Materials Science and Chemical Engineering

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

University of California, Department of Botany & Plant Sciences

University of California, Davis, Department of Chemistry

University of California, Irvine, Department of Chemistry, Department of Molecular Biology and Biochemistry

University of Michigan, Department of Chemical Engineering

University of Pennsylvania, Department of Materials Science and Engineering

University of Wisconsin, Milwaukee, Department of Chemistry and Biochemistry

*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

Yukimoto, M.
Creation of Tautomerizable Heavy Group 14–16 Double Bonded Compounds
Grant-in-Aid for Early-Career Scientists
1 April 2019–31 March 2022

Tokitoh, N.
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

— Structural Organic Chemistry —

Murata, Y.
Creation and Development of Nanoscale Laboratory
Grant-in-Aid for Scientific Research (S)
31 May 2017–31 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 Areas (Research in a Proposed Research Area)
1 April 2020–31 March 2022

Hirose, T.
Synthesis of π -Extended Helical Aromatic Molecules Towards Creation of Nobel 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 Areas (Research in a Proposed Research Area)
1 April 2019–31 March 2021

Zhang, S.
Creation of Expanded and Heteroatom-Embedded New Fullerenes
Grant-in-Aid for JSPS Fellows
11 October 2019–31 March 2022

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

Hirose, T.
Creation of Asymmetric Molecular Functions Based on the Precise Molecular Arrangements of Helical π -Conjugated Compounds
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 December 2020–31 March 2024

— Synthetic Organic Chemistry —

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

Ueda, Y.
Sugar-Specific Chemical Transformation towards Diversification of Synthetic Sugar Library
Grant-in-Aid for Transformative Research Areas (B)
23 August 2021–31 March 2024

Kawabata, T.
Asymmetric Construction of Interlocked Molecules by Remote Asymmetric Induction
Grant-in-Aid for Scientific Research (B)
1 April 2021–31 March 2024

— Advanced Inorganic Synthesis —

Teranishi, T.
Novel Development of Asymmetry Chemistry in Inorganic Nanocrystals
Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area)
30 June 2016–31 March 2021

Sato, R.
Scientific Principles of Visible Plasmonic Nanoalloys
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 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

Sakamoto, M.
Infrared Light Responsive Photocatalyst for Infrared Light to Energy Conversion
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 March 2022

Liu, M.-H.
Fabrication of Visible-Light Driven Heterostructured Cu₂O/Au/WO₃ Photocatalyst for Water Splitting
Grant-in-Aid for JSPS Fellows
12 October 2018–31 March 2021

Teranishi, T.
Nanoscale Metallic Phase Science: Synthesis of Nanoparticles with Novel Metallic Phases and Development of Their Functions
Grant-in-Aid for Scientific Research (A)
1 April 2019–31 March 2022

Trinh, T.
Evolution of New Magnetic Materials with Ultrahigh Coercivity
Grant-in-Aid for Early-Career Scientists
1 April 2019–31 March 2022

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.
Synthesis of Unprecedented Ordered Alloy Nanoparticles and Development of Their Structure-Specific Properties
Grant-in-Aid for Challenging Research (Exploratory)
28 June 2019–31 March 2021

Sakamoto, M.
Clear and Transparent Device for Infrared Light to Energy Conversion using Heavily Doped Semiconductor Nanocrystals
Grant-in-Aid for Challenging Research (Exploratory)
28 June 2019–31 March 2021

Saruyama, M.
Synthesis and Function of Versatile 3-Dimensional Inorganic Nanocrystal Superlattice
Grant-in-Aid for Challenging Research (Exploratory)
30 July 2020–31 March 2023

Sakamoto, M.
Fabrication of Flexible Transparent Conductive Films using Nanocrystals
A-STEP (Adaptable and Seamless Technology Transfer Program through Target-Driven R&D), JST
1 December 2020–31 March 2023

Sakamoto, M.
Development of Transparent Solar Cells Converting Infrared Light
Fusion Oriented Research for Disruptive Science and Technology
1 January 2021–31 March 2023

Sakamoto, M.
Development of Energy Conversion System of Untapped Infrared Solar Light
Grant-in-Aid for Scientific Research (A)
5 April 2021–31 March 2026

Teranishi, T.
Creation of Unprecedented Nanomaterials by Arranging Atomic Layers and Crystal Phases
CREST (Core Research for Evolutionary Science and Technology), JST
1 October 2021–31 March 2027

DIVISION OF MATERIALS CHEMISTRY **— Chemistry of Polymer Materials —**

Ohno, K.
Ordered Structure Formation in Polymer-Brush-Decorated-Particle/Liquid-Crystal Mixed System
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 March 2021

Sakakibara, K.
Molecular Design of Polymer Dispersants for the Improvement of Toughness of Cellulose Nanofiber-Reinforced Resin Composite Materials
Grant-in-Aid for Scientific Research (C)
1 April 2019–31 March 2022

Tsujii, Y.
Development of High-Performance Sliding Components with Concentrated Polymer Brushes and Their Application to Machines A-STEP (Adaptable and Seamless Technology Transfer Program through Target-Driven R&D), JST
1 December 2020–31 March 2025

Ohno, K.
Construction of Colloidal Crystals with Simple Cubic Lattice by Precisely Designed Polymer-Brush-Decorated Hybrid Particles
Grant-in-Aid for Scientific Research (B)
1 April 2021–31 March 2024

Tsujii, Y.
Hierarchical Understanding and Control of Wear Behavior of Ultralow-Friction Polymer Brushes
CREST (Core Research for Evolutionary Science and Technology), JST
1 October 2021–31 March 2027

— Polymer Controlled Synthesis —

Yamago, S.
New Organic Chemistry and Materials Science of Curved π -Conjugated Molecules
Grant-in-Aid for Scientific Research (S)
31 May 2016–31 March 2021

Yamago, S.
Development of Next-Generation Polymer Materials Based on Hyper-Branched Polymers with Controlled Structures
Grant-in-Aid for Scientific Research (S)
5 July 2021–31 March 2026

— Inorganic Photonics Materials —

Mizuochi, N.
Advanced Sensor System of Solid Quantum Sensor in Quantum Measurement and System Technology
OPERA (Program on Open Innovation Platform with Enterprises, Research Institute and Academia)
1 August 2018–31 March 2030

Mizuochi, N.
Creation of Innovative Sensor System by Advanced Control of Solid-State Quantum Sensor in Development of Quantum Measurement Sensing Technology
Q-LEAP (Quantum Leap Flagship Program), MEXT
1 November 2018–31 March 2028

Mizuochi, N.
Creation of Quantum Life Technology and Innovation in Medicine and Life Sciences
Q-LEAP (Quantum Leap Flagship Program), MEXT
31 August 2020–31 March 2030

— Nanospintronics —

Shiota, Y.
Control of Antiferromagnetic Spin Waves in Synthetic Antiferromagnets
Grant-in-Aid for Early-Career Scientists
1 April 2020–31 March 2022

Ono, T.
Ferrimagnetic Spintronics and Their Devices
Grant-in-Aid for Scientific Research (S)
31 August 2020–31 March 2025

Moriyama, T.
Spin Superfluid in Antiferromagnetic Thin Films
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 December 2020–31 March 2024

Narita, H.
Control of Superconductivity by Noncollinear Magnetism
Grant-in-Aid for Early-Career Scientists
1 April 2021–31 March 2024

Moriyama, T.
Antiferromagnetic THz Spintronics
Grant-in-Aid for Scientific Research (A)
5 April 2021–31 March 2024

Ono, T.
Development of 3D Magnetic Memory
CREST (Core Research for Evolutionary Science and Technology), JST
1 October 2021–31 March 2027

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

Imanishi, M.
Control of RNA Modification for Antivirus Activities
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

Futaki, S.
Development of New Methods for in vivo Delivery of Antibodies to Intracellular Targets
Grant-in-Aid for Scientific Research (A)
5 April 2021–31 March 2024

— 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 Areas (Research in a Proposed Research Area)
30 June 2017–31 March 2022

Mashiguchi, K.
Analysis of the Novel Enzymes Responsible for the Non-Canonical Strigolactone Biosynthesis
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2024

— Molecular Biology —

Kato, M.
Study of Phosphoinositides Involved in Pollen Germination
Grant-in-Aid for Scientific Research (C)
1 April 2021–31 March 2025

Aoyama, T.
Role of Phosphoinositide Signals in Plant Cell Morphogenesis
Grant-in-Aid for Scientific Research (B)
1 April 2021–31 March 2024

— Chemical Biology —

Uesugi, M.
Frontier Research on Chemical Communications
Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area)
30 June 2017–31 March 2022

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

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

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

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

Sato, S.
A New Oligonucleotide Therapeutics that Induces a Cooperative RNA G-Quadruplex Formation for Gene Silencing
Grant-in-Aid for Challenging Research (Pioneering)
9 July 2021–31 March 2025

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

Uesugi, M.
Self-Assembling Vaccine Adjuvants
A-STEP (Adaptable and Seamless Technology Transfer Program
through Target-Driven R&D), JST
1 April 2021–31 March 2022

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

Sato, S.
Development of Nucleic-Acid-Medicine Mechanisms by Staple
Oligomer
AMED Research on Development of New Drugs
1 October 2021–31 March 2024

Takemoto, Y.
Elucidation of the Mechanism of Energy Metabolism by Vitamin
D Lactone
Mishima Kaiun Memorial Foundation
1 September 2021–30 June 2022

Takemoto, Y.
Understanding and Application of Radical-Sensitive Peptide
Takeda Science Foundation
1 September 2021–31 May 2024

DIVISION OF ENVIRONMENTAL CHEMISTRY

— Molecular Materials Chemistry —

Suzuki, K.
Structural Analysis of Organic Semiconducting Materials Using
Solid-State NMR
Grant-in-Aid for Early-Career Scientists
1 April 2019–31 March 2022

Shizu, K.
Singlet Fission Materials by Engineering Inter-Exciton Vibronic
Coupling
Grant-in-Aid for Scientific Research (C)
1 April 2019–31 March 2022

Kaji, H.
Material Design Based on Dynamic Excitation and Their Applica-
tions
Grant-in-Aid for Transformative Research Areas (A)
19 November 2020–31 March 2025

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

— Hydrospheric Environment Analytical Chemistry —

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

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

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

— Chemistry for Functionalized Surfaces —

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
1 April 2019–31 March 2022

Hasegawa, T.
Development of Property Control of Polymer Thin Materials by
Analyzing Minute Morphology of Amorphous Parts
Grant-in-Aid for Challenging Research (Exploratory)
9 July 2021–31 March 2024

— Molecular Microbial Science —

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

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

Kurihara, T.
Dissection of the Molecular Basis of Membrane Vesicle Biogen-
esis 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.
Molecular Basis for Generation of the Diversity of Bacterial
Membrane Phospholipid Acyl Chains and Mechanisms Underly-
ing their Physiological Functions
Grant-in-Aid for Scientific Research (B)
1 April 2021–31 March 2024

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

Ogawa, T.
Research on the Metabolic Conversion of ω -3 Polyunsaturated
Fatty Acids through Reconsideration of β -Oxidation Pathway
Grant-in-Aid for Scientific Research (C)
1 April 2021–31 March 2024

DIVISION OF MULTIDISCIPLINARY CHEMISTRY

— Polymer Materials Science —

Takenaka, M.
4D Analysis of Grazing Incidence Scattering for Investigation of Adhesion Process at Adhesive Interface
Mirai Program, JST
1 November 2018–31 March 2022

Ogawa, H.
Development of Multibeam Optics for Scanning CT
CREST (Core Research for Evolutionary Science and Technology), JST
1 April 2021–31 March 2022

— Molecular Rheology —

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

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

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

— 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
1 April 2016–31 March 2021

Truong, M. A.
Efficient Perovskite Solar Cells Based on Development of Transparent Organic Semiconductors
Grant-in-Aid for JSPS Fellows
12 October 2018–31 March 2021

Murdey, R.
Aging and Passivation Effects in Perovskite Solar Cells
Grant-in-Aid for Scientific Research (C)
1 April 2019–31 March 2022

Nakamura, T.
Emissive Perovskite Materials for Blue Electroluminescence Devices
Grant-in-Aid for Research Activity Start-up
30 August 2019–31 March 2021

Truong, M. A.
Development of Charge Collecting Materials for High Performance Sn-based Perovskite Solar Cells
Grant-in-Aid for Research Activity Start-up
11 September 2020–31 March 2022

Nakamura, T.
Two-Dimensionally Expanded pi-Systems for Efficient Tin-Based Perovskite Solar Cells
Grant-in-Aid for Early-Career Scientists
1 April 2021–31 March 2023

Wakamiya, A.
Fundamental Chemical Research for Efficient Pb Free Perovskite Solar Cells
Grant-in-Aid for Scientific Research (A)
5 April 2021–31 March 2024

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE

— Particle Beam Science —

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

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

Wakasugi, M.
Development of Unstable Nuclear Target for Nuclear Reaction Study
Grant-in-Aid for Challenging Research (Pioneering)
1 April 2020–31 March 2022

— Electron Microscopy and Crystal Chemistry —

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

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

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

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Synthetic Organotransformation —

Nakamura, M.
Application and Evaluation of Quantum Effect Control in Iron-Catalyzed Cross Coupling
Grant-in-Aid for Scientific Research (B)
1 April 2020–31 March 2023

Takaya, H.
Development of Metalated Peptide Artificial Enzymes for Utilizing Woody Biomass as Circulative Resource
Grant-in-Aid for Scientific Research (C)
1 April 2021–31 March 2024

— **Advanced Solid State Chemistry** —

Shimakawa, Y.
Solid State Chemistry of Transition Metal Oxides: Exploration of New Materials and Innovative Functions
Core-to-Core Program, JSPS
1 April 2016–31 March 2021

Shimakawa, Y.
High-Pressure Synthesis of Novel Transition Metal Oxides and Exploration of New Physical Properties
Grant-in-Aid for Scientific Research (A)
1 April 2020–31 March 2024

Shimakawa, Y.
Development of New Multi-Calorific Materials
Grant-in-Aid for Challenging Research (Pioneering)
30 July 2020–31 March 2024

— **Organometallic Chemistry** —

Ohki, Y.
Synthesis and Reactions of Mo-Fe-S Clusters Toward Understanding of the Mechanism of Nitrogenase
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

Ohki, Y.
Synthesis of Metal-Nanoclusters of Iron Group Metals
Grant-in-Aid for Challenging Research (Exploratory)
30 July 2020–31 March 2023

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

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

Wakioka, M.
Study on True Correlation of Primary Structure and Charge Transport Property for pi-Conjugated Polymers
Grant-in-Aid for Scientific Research (C)
1 April 2021–31 March 2024

Tanifuji, K.
Structure-Function Relationships of Fe-Mo-S-C Metallocofactor of Dinitrogen-Reducing Enzymes
Grant-in-Aid for Research Activity Start-up
30 August 2021–31 March 2023

— **Nanophotonics** —

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

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

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

BIOINFORMATICS CENTER

— **Chemical Life Science** —

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

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

Ogata, H.
Deciphering the Mechanisms of Virus-Host Co-Existence in Aquatic Environments
Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area)
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 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

Okazaki, Y.
Microbial Nitrogen Pump: Bacterial Semi-Labile Dissolved Organic Nitrogen as a Nutrient Transport Pathway in Aquatic Systems

Grant-in-Aid for Scientific Research (B)
1 April 2021–31 March 2024

Okazaki, Y.
Prokaryotic Genomic Microdiversity Revealed Through Cutting-Edge Ecogenomics
The Kyoto University Foundation
16 June 2021–31 March 2022

Endo, H.
Change in Ecological Stoichiometry of Marine Phytoplankton Driven by Symbiotic Interaction and Its Mechanisms
Mitsumasa Ito Memorial Research Grant, Research Institute for Oceanography Foundation
1 April 2021–31 March 2022

Ogata, H.
Grant for Holding International Conferences
The Kyoto University Foundation
1 April 2021–31 March 2022

Ogata, H.
Elucidation of the Virus-Driven Clockwork of the Marine Lower Trophic Level Ecosystem and Its Influence on Our Ocean
Grant-in-Aid for Scientific Research (S)
1 April 2021–31 March 2026

— **Mathematical Bioinformatics** —

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

Mori, T.
Development of Cell Trajectory Inference and Comparison Algorithm Based on Single-Cell Omics Data
Grant-in-Aid for Early-Career Scientists
1 April 2019–31 March 2022

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

— **Bio-knowledge Engineering** —

Mamitsuka, H.
Development of Next Generation Plastic Materials Based on Structurally Controlled Hyperbranched Polymers
Grant-in-Aid for Scientific Research (S)
5 July 2021–31 March 2026

Mamitsuka, 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

Petschner P.
Developing Machine Learning Based Bioinformatics to Decipher Hidden Biology of Depression Symptoms
Grant-in-Aid for JSPS Fellows
13 November 2020–31 March 2023

Mamitsuka, H.
Deep Learning of Mechanistic Networks in Cellular Signaling from Experimental Data
Research Support Allowance, JSPS
15 March 2021–13 May 2021

THESES

- CHEN, Gong
D Pharm Sc, Kyoto University
“Studies on Chemo- and Site-Selective C-H Amination of Aniline and Phenol Derivatives with Dirhodium Catalysts and Catalytic Asymmetric Synthesis of Inherently Chiral Calixarenes”
Supervisor: Prof KAWABATA, Takeo
24 March 2021
- HAKARIYA, Hayase
D Med Sc, Kyoto University
“Non-Genetic Cell-Surface Modification with a Self-Assembling Molecular Glue”
Supervisor: Prof UESUGI, Motonari
23 March 2021
- HIRATA, Yuushou
D Sc, Kyoto University
“Compensation Temperature in GdFe Alloys and Magnetic Domain Wall Creep in Tb/CoFeB”
Supervisor: Prof ONO, Teruo
19 January 2021
- ISHIBASHI, Mio
D Sc, Kyoto University
“Spin Waves in Synthetic Antiferromagnets”
Supervisor: Prof ONO, Teruo
19 January 2021
- IWAI, Kento
D Sc, Kyoto University
“Synthesis and Properties of Zwitterionic Compounds Utilizing an Introducing Unit of a Boranuidyl Group”
Supervisor: Prof TOKITOH, Norihiro
23 March 2021
- JIN, Masayoshi
D Eng, Kyoto University
“Development of Iron-Catalyzed Enantioselective Carbon-Carbon Bond Forming Reactions for Efficient Access to Bioactive Compounds and Their Derivatives”
Supervisor: Prof NAKAMURA, Masaharu
24 November 2021
- KINOSE, Yuji
D Eng, Kyoto University
“Fundamental and Applied Studies on Molecular Bottlebrushes with Particular Reference to Side-Chain Conformation and Dynamics”
Supervisor: Prof TSUJII, Yoshinobu
23 March 2021
- KOEDTRUAD, Anucha
D Sc, Kyoto University
“Synthesis of Novel Metal Halides and Their Structure-Property Relations”
Supervisor: Prof SHIMAKAWA, Yuichi
24 March 2021
- KURODA, Ryo
D Sc, Kyoto University
“Functions of the *Arabidopsis thaliana* PIP5K Genes, *PIP5K7*, *PIP5K8*, and *PIP5K9*”
Supervisor: Prof AOYAMA, Takashi
24 May 2021
- LAI, Ming-Wei
D Sc, Kyoto University
“Investigation of Ordered Structures in Oxidation-Synthesized α -Fe₂O₃ Nanowhiskers with Cs-Corrected HR-TEM and Monochromated Core-Loss EELS”
Supervisor: Prof KURATA, Hiroki
24 September 2021
- LI, Tien
D Sc, Kyoto University
“Spin Wave Propagation in Ferromagnetic Nano-Structures”
Supervisor: Prof ONO, Teruo
19 January 2021
- LI, Xiaopei
D Eng, Kyoto University
“Elucidation of the Termination Reaction Mechanism of Radical Polymerization”
Supervisor: Prof YAMAGO, Shigeru
23 March 2021
- LI, Zhanzhao
D Sc, Kyoto University
“Transformative Inorganic Nanocrystals during Cation Exchange Reaction”
Supervisor: Prof TERANISHI, Toshiharu
12 November 2021
- LIU, Pengyu
D Inf, Kyoto University
“Extracting Rules from Trained Machine Learning Models with Applications in Bioinformatics”
Supervisor: Prof AKUSTU, Tastuya
24 May 2021
- MARUOKA, Naruyuki
D Agr, Kyoto University
“Studies on a Bioactive Substance for Epidermal Barrier Improvement Derived from Fermented Barley Extract”
Supervisor: Prof KURIHARA, Tatsuo
24 November 2021
- NINOMIYA, Ryo
D Pharm Sc, Kyoto University
“Development of Synthetic Method for α -Chiral Amines Based on C-H Functionalization”
Supervisor: Prof KAWABATA, Takeo
24 March 2021
- NISHIYAMA, Hiroki
D Pharm Sc, Kyoto University
“Characterization of Features of Gut Microbiota Related to Gut Homeostasis and Disease Progression”
Supervisor: Prof OGATA, Hiroyuki
23 March 2021

OMATSU, Yamato
D Sc, Kyoto University
“Synthetic Study on Functionalized Oligosilanes toward Aromatic Silicon Clusters”
Supervisor: Prof TOKITOH, Norihiro
23 March 2021

SAKAMOTO, Kentarou
D Pharm Sc, Kyoto University
“Cytosolic Delivery of Macromolecules by Peptides and Peptide Nanocarrier”
Supervisor: Prof FUTAKI, Shiroh
23 March 2021

SANARI, Yasuyuki
D Sc, Kyoto University
“High-Order Harmonic Generation and Nonlinear Current Dynamics in Solids”
Supervisor: Assoc Prof HIRORI, Hideki
23 March 2021

TAN, Zhenhong
D Sc, Kyoto University
“High-Pressure Synthesis and Properties of Novel Hexagonal Perovskites Containing Unusual High-Valence Fe Ions”
Supervisor: Prof SHIMAKAWA, Yuichi
24 March 2021

XING, Yongning
D Pharm Sc, Kyoto University
“Synthetic Studies of Amide-Functionalized Helicene-Like Molecules”
Supervisor: Prof KAWABATA, Takeo
24 May 2021



**THE 121ST
ICR ANNUAL
SYMPOSIUM**

SEMINARS

**MEETINGS AND
SYMPOSIA**



THE 121ST ICR ANNUAL SYMPOSIUM

(10 December 2021)

ORAL PRESENTATION

TAKEMOTO, Yasushi (Chemical Biology)
“Chemical Biology Reveals New Functions of Squalene Synthase”

OHNO, Kohji (Chemistry of Polymer Materials)
“Self-Assembly of Polymer-Brush-Decorated Hybrid Particles”

AOYAMA, Takashi (Molecular Biology)
“Genetic Analysis of Plant Phosphoinositide Signaling”

OGAWARA, Ryo (Particle Beam Science)
“Development of Resonant-Extraction Charge Breeder for Nuclear Reaction Studies of Rare-RP”

ENDO, Hisashi (Chemical Life Science)
“Biogeography of Marine Phytoplankton”

— ICR Award for Young Scientists —

ENDO, Hisashi (Chemical Life Science)
“Biogeography of Marine Giant Viruses Reveals Their Interplay with Eukaryotes and Ecological Functions”

— ICR Award for Graduate Students —

IWATA, Takahiro (Biofunctional Design-Chemistry)
“Liquid Droplet Formation and Facile Cytosolic Translocation of IgG in the Presence of Attenuated Cationic Amphiphilic Lytic Peptides”

LI, Zhanzhao (Advanced Inorganic Synthesis)
“Determinants of Crystal Structure Transformation of Ionic Nanocrystals in Cation Exchange Reactions”

KOSUGI, Yoshihisa (Advanced Solid State Chemistry)
“Gigantic Barocaloric Effect by Large Latent Heat Produced by First-Order Intersite-Charge-Transfer Transition”

— ICR Grants for Promoting Integrated Research —

NAKAMURA, Tomoya (Molecular Aggregation Analysis)
“Efficient Perovskite Solar Cells Using Structural Analysis by Infrared Spectroscopy”

AMANO PATINO, Midori Estefani (Advanced Solid State Chemistry)
“Investigation of Oxide Ion Mobility in a Series of Ruddlesden-Popper Perovskite Derivatives”

HAYASHI, Kan (Nanophotonics)
“Spatially Controlled Fabrication of Shallow Nitrogen-Vacancy Centers in Diamond”

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”

GE GARCIA, Julius Adrie; YUKIMOTO, Mariko; MIZUHATA, Yoshiyuki; TOKITOH, Norihiro
“A Novel 1,4-Silyl Group Migration in the Reaction of a Sterically Hindered Benzylic Telluride with an Alkylolithium”

— Structural Organic Chemistry —

LW “Research Activities in Structural Organic Chemistry Laboratory”

GE ZHANG, Sheng; HASHIKAWA, Yoshifumi; MURATA, Yasujiro
“Cage-Expansion of Fullerenes”

— Synthetic Organic Chemistry —

LW “Current Topics in Laboratory of Synthetic Organic Chemistry”

— Advanced Inorganic Synthesis —

LW “Research in Advanced Inorganic Synthesis”

GE SUZUKI, Wataru; TAKAHATA, Ryo; TERANISHI, Toshiharu
“Control over the Reactivity of Ligand-Exchange Reactions of a Gold Nanocluster by Bulky Incoming Ligands”

— Chemistry of Polymer Materials —

LW “Recent Research in Chemistry of Polymer Materials Laboratory”

GE TAKAMURA, Yoshiro; KINOSE, Yuji; TSUJII, Yoshinobu
“Anchoring Property of Liquid Crystal on Structurally Controlled Bottlebrush Thin Film”

— Polymer Controlled Synthesis —

LW “Research Activities in Laboratory of Polymer Controlled Synthesis”

GE GOTO, Kana; TOSAKA, Masatoshi; YAMAGO, Shigeru
“Elucidation of the Branching Effect in the Conformations of Amphiphilic Diblock Copolymers with Multibranching Structures”

[GE] ZHU, Nanyi; TOSAKA, Masatoshi; YAMAGO, Shigeru
“Understanding and Predicting Monomer Reactivity Ratios in Radical co-Polymerization Using Machine Learning”

[GE] MORI, Takahiro; KAYAHARA, Eiichi; KATO, Tatsuhisa; YAMAGO, Shigeru
“Synthesis and In-Plane Aromaticity of Dianion of Cyclic Paraphenylene Diketone”

— Inorganic Photonics Materials —

[LW] “Research Activities in Laboratory of Inorganic Photonics Materials”

— Nanospintronics —

[GE] FUNADA, Shinsaku
“Temperature Dependence of the Magnetic Damping Constant in Ferromagnetic Garnet $Gd_3Fe_5O_{12}$ Film”

— Biofunctional Design-Chemistry —

[LW] “Research in the Biofunctional Design Chemistry Laboratory”

[GE] OTONARI, Kenko; SHINODA, Kouki; IMANISHI, Miki; FUTAKI, Shiroh
“Development and Perspective of Sequence-Specific RNA Demethylase”

— Chemistry of Molecular Biocatalysts —

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

— Molecular Biology —

[LW] “Research Activities in Molecular Biology Laboratory”

— Chemical Biology —

[LW] “Create New World of Bioactive Synthetic Molecules”

— Molecular Materials Chemistry —

[LW] “Molecular Materials Chemistry”

[GE] REN, Yongxia; WADA, Yoshimasa; SUZUKI, Katsuaki; KUSAKABE, Yu; GELDSETZER, Jan; KAJI, Hironori
“A Novel Blue Thermally Activated Delayed Fluorescence Emitter Possessing Very Fast Reverse Intersystem Crossing”

[GE] MURAMATSU, Tomomi; TANAKA, Hiroyuki; SUZUKI, Katsuaki; KAJI, Hironori
“Development of Solution-Processable Red Thermally Activated Delayed Fluorescence Materials”

— Hydrospheric Environment Analytical Chemistry —

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

[GE] MATSUOKA, Kohei; TATSUYAMA, Tomomichi; TAKANO, Shotaro; SOHRIN, Yoshiki
“Origin Analysis Using Stable Isotope Ratios of Mo and W in the Hydrosphere”

— Chemistry for Functionalized Surfaces —

[GE] YOSHIDA, Mariko; SHIOYA, Nobutaka; TOMITA, Kazutaka; SHIMOAKA, Takafumi; HASEGAWA, Takeshi
“Template-Free Control of Molecular Orientation in Ph-BTBT- C_{10} Thin Films”

[GE] OOTSUKI, Masashi; SHIMOAKA, Takafumi; SHIOYA, Nobutaka; HASEGAWA, Takeshi
“Visualization of Molecular Orientation in Perfluoroalkane Particles by Raman Microscope Spectroscopy”

— Molecular Microbial Science —

[LW] “Introduction of Molecular Microbial Science Laboratory”

[GE] ZHU, Mengshan; OGAWA, Takuya; KAWAMOTO, Jun; IMAI, Tomoya; KURIHARA, Tatsuo
“Construction of Hypervesiculation Mutants of *Shewanella vesiculosa* HM13 by Disrupting Genes Involved in Outer Membrane-Peptidoglycan Linkage”

— Polymer Materials Science —

[LW] “Polymer Materials Science”

[GE] AOKURA, Shuta; TAKENAKA, Mikihiro
“Universality of Strain-Induced Density Fluctuations in Glassy Materials”

[GE] KUWATA, Satoshi
“Evaluation of Heterogeneity of Nano-Scale Structure in Epoxy Adhesives by SMAXS-CT Method”

—Molecular Rheology —

[LW] “Research Activities in Molecular Rheology Laboratory”

— Molecular Aggregation Analysis —

[LW] “Research in Molecular Aggregation Analysis”

[GE] TRUONG, Minh Anh; UEBERRICKE, Lucas; FUNASAKI, Tsukasa; NOJO, Wataru; MURDEY, Richard; NAKAMURA, Tomoya; SUZUKI, Takanori; WAKAMIYA, Atsushi
“Development of Hole-Collecting Monolayer Materials Based on Triazatruxene Skeleton”

[GE] HU, Shuaifeng; OTSUKA, Kento; MURDEY, Richard; NAKAMURA, Tomoya; TRUONG, Minh Anh; YAMADA, Takumi; HANDA, Taketo; MATSUDA, Kazuhiro; NAKANO, Kyohei; SATO, Atsushi; MARUMOTO, Kazuhiro; TAJIMA, Keisuke; KANEMITSU, Yoshihiko; WAKAMIYA, Atsushi
“Mixed Tin-Lead Perovskite Solar Cells Achieved 23.6% Efficiency”

— Particle Beam Science —

[LW] “Particle Beam Science Laboratory”

— Laser Matter Interaction Science —

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

— Electron Microscopy and Crystal Chemistry —

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

[GE] LIN, I-Ching; HARUTA, Mitsutaka; NEMOTO, Takashi; KURATA, Hiroki
“Structural Sensitivity and Atomic Vibration Effect on Ti $L_{2,3}$ -Edge Core-Excited Spectrum”

— Atomic and Molecular Structures —

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

— Synthetic Organotransformation —

[LW] “Introduction of Synthetic Organotransformation Group”

[GE] SUZUKI, Shogo; NAKAMURA, Yuki; ISOZAKI, Katsuhiro; NAKAMURA, Masaharu
“Development of Organoacid Catalysts to Facilitate Woody Biomass Degradation Reaction”

[GE] ISERI, Kenta; ISOZAKI, Katsuhiro; NAKAMURA, Masaharu
“Dual Catalysis of Peptide Dendron-Functionalized Gold Nanoclusters toward α -C-H Alkynylation of Aliphatic Amines”

[GE] LU, Siming; AGATA, Ryosuke; ISOZAKI, Katsuhiro; NAKAMURA, Masaharu
“Iron-Catalyzed Cross Coupling of Propargyl Electrophiles with Organoboron Reagents”

— Advanced Solid State Chemistry —

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

— Organometallic Chemistry —

[LW] “Recent Research Topics of the Ohki Laboratory”

[GE] WAKIOKA, Masayuki; ISHIZUKA, Risa
“Properties of Polythiénylenevinylenes with Short Alkyl Side Chains”

[GE] SAKAI, Yuta; TANIFUJI, Kazuki; TADA, Mizuki; OHKI, Yasuhiro
“ N_2 Reduction by the Co Sites Incorporated into Incomplete-Cubane $[Mo_3S_4]$ Cores”

— Nanophotonics —

[LW] “Recent Research Topics of Nanophotonics Group”

— Chemical Life Science —

[LW] “Laboratory of Chemical Life Science”

— Mathematical Bioinformatics —

[LW] “DynCubeProd: Dynamic Solution Space Division-Based Methods for Calculating Reaction Deletion Strategies for Constraint-Based Metabolic Networks for Substance Production”

— Bio-knowledge Engineering —

[LT] NGUYEN, Canh Hao; MAMITSUKA, Hiroshi
“Convex Clustering: Convexity, Bounding Balls and General Characteristics”

SEMINARS

Prof ASANO, Yasuhiro
Department of Applied Physics, Hokkaido, Japan
“Andreev Reflection and Josephson Junctions”
25 June 2021

Prof HANAMOTO, Takeshi
Faculty of Science and Engineering, Saga University, Saga, Japan
“Synthesis and Derivatization of Fluorovinylsulfonium Salts”
29 January 2021

Prof HAYES, Paul
Department of Chemistry and Biochemistry and Canadian
Centre for Research in Advanced Fluorine Technologies, Univer-
sity of Lethbridge, Lethbridge, Canada
“Metal-Ligand Cooperative Small Molecule Activation by
Rhodium NNN-Pincer Complexes”
30 August 2021

Assoc Prof KONDO, Yoshiko
Graduate School of Fisheries and Environmental Sciences, Nagasaki
University, Nagasaki, Japan
“Dynamics of Trace Metals such as Fe in the Ocean”
3 December 2021

Prof MASUBUCHI, Yuichi
Nagoya University, Aichi, Japan
“Relationship between Strength of Tetra-PEG Gel and Molecular
Weight Distribution of Prepolymer Studied by Simulation”
17 December 2021

Prof NAKAJIMA, Atsushi
Department of Chemistry, Faculty of Science and Technology,
Keio University, Tokyo, Japan
“Creation and Characterization of Silicon-Cage Nanoclusters”
18 November 2021

Prof OKADA, Mariko
Institute for Protein Research, Osaka University (Visiting Profes-
sor of Bioinformatics Center), Osaka, Japan
“Mathematical Modeling of Cancer Signaling Networks for
Patient Classification”
30 March 2021

Prof ORITA, Akihiro
Faculty of Engineering, Okayama University of Science, Okayama,
Japan
“Reductive Desulfonylation by Organophotocatalysis”
26 February 2021

Prof SAKAI, Takamasa
The University of Tokyo, Tokyo, Japan
“Understanding the Science of Dilute Polymeric Networks”
17 December 2021

Prof SASAMORI, Takahiro
University of Tsukuba, Ibaragi, Japan
“X-Ray Crystal Structure Analysis”
27 September 2021

Dr SOHTOME, Yoshihiro
RIKEN Cluster for Pioneering Research, Saitama, Japan
“Dynamic Catalysis: Toward Symbiosis between Molecular
Catalysts and Enzymes”
1 March 2021

Prof TAKIMOTO, Jun-ichi
Yamagata University, Yamagata, Japan
“Simulation Study of High-Speed Flow of Unentangled Polymers”
17 December 2021

Assoc Prof UNEYAMA, Takashi
Nagoya University, Aichi, Japan
“Static and Dynamic Shielding Effects of Interaction in Interacting
Dumbbell Systems”
17 December 2021

Assoc Prof URAKAWA, Osamu
Department of Macromolecular Science, Graduate School of
Science, Osaka University, Osaka, Japan
“Dynamics of Polymer Systems with Specific Interactions”
17 December 2021

Prof URAYAMA, Kenji
Kyoto Institute of Technology, Kyoto, Japan
“Elucidation of Crack Properties of Elastomers in Biaxial
Elongation Fields”
17 December 2021

MEETINGS AND SYMPOSIA

Asian Chemical Biology Initiative 2021 Online Meeting

Organized by UESUGI, Motonari
24-25 February 2021 (Online)

SRT Symposium

Organized by TSUJII, Yoshinobu
17 March 2021 (Kyoto, Japan)

Physiological Functions of Bacterial Extracellular Membrane Vesicles and the Mechanism of Their Biogenesis

Organized by KURIHARA, Tatsuo
20 March 2021 (Online, Miyagi, Japan)

Aquatic Virus Workshop 10

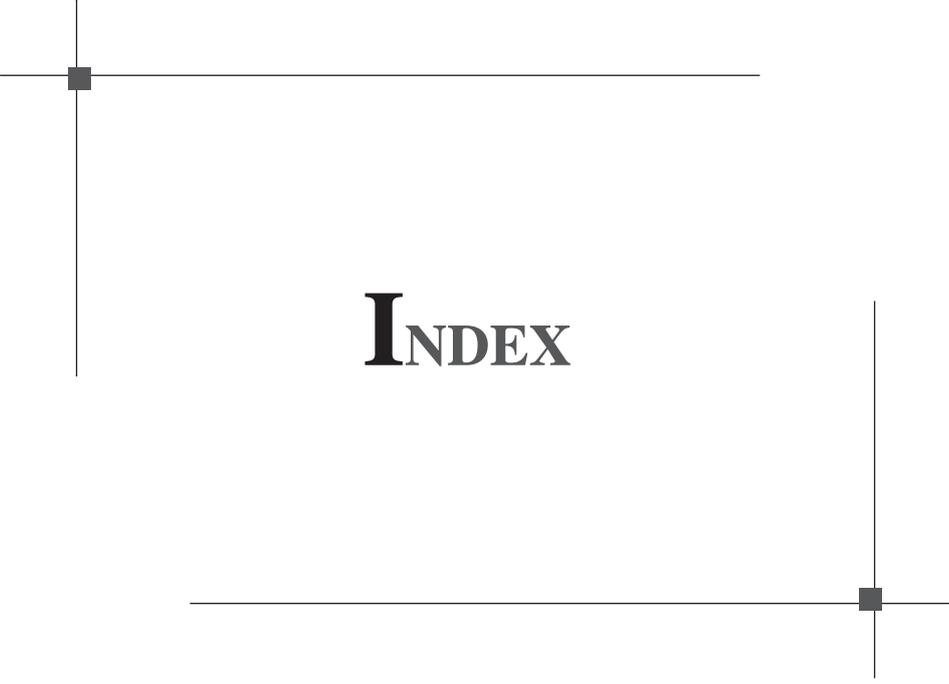
Organized by OGATA, Hiroyuki
27 June-1 July 2021 (Kyoto, Japan)

75th Annual Autumn Meeting of the Research Institute for Ocean Chemistry Foundation

Organized by SOHRIN, Yoshiki
13 November 2021 (Kyoto, Japan)

The 5th MAIRS Workshop

Organized by HASEGAWA, Takeshi
19 November 2021 (Kyoto, Japan)



INDEX

NAME INDEX

[A]		[H]		IWASE, Misato	30
ABO, Masahiro	26	HAGHIR, Shahrzad	24	IWASHIMIZU, Chisaki	46
ADO, Genyir	26	HARA, Yuta	36	IWATA, Takahiro	20, 81
AKAGI, Chika	24	HARIKI, Nene	16	[J]	
AKUTSU, Tatsuya	60	HARUTA, Mitsutaka	46	JIANG, Yuhan	14
AMANO PATINO, Midori Estefani	52	HASEGAWA, Takeshi	32	JIN, Shuyu	26
AOKURA, Syuta	36	HASHIDA, Masaki	44	JUNG, Yejin	26
AOYAMA, Takashi	24	HASHIKAWA, Yoshifumi	6	JUN-I, Yuta	4
ARAKAWA, Masato	36	HASHIMOTO, Hisashi	8	[K]	
ASAMI, Yuri	20	HASHIMOTO, Kentaro	58	KAJI, Hironori	28
AVENA, Ramon Francisco Bernardino	50	HASHIMOTO, Ruito	40	KAMADA, Taro	52
[B]		HAYASHI, Kan	56	KAMASAKA, Kouhei	34
BAN, Hiroki	58	HERBSCHLEB, Ernst David	16	KAN, Daisuke	52
[C]		HIKIDA, Hiroyuki	58	KANAMURA, Hideo	30
CHAN, Cheuk-Yin	30	HIRA, Shota	6	KANDA, Kazuaki	4
CHEN, Jingjie	58	HIRAI, Yusuke	20	KANDA, Syun	28
CHEN, Litian	50	HIRANO, Toshiko	4	KANEHISA, Minoru	76
CHIGA, Yuki	10	HIRASHIMA, Maho	34	KANEKO, Hiroto	58
CHO, Kenichi	56	HIRATA, Saya	14	KANEKO, Ryuji	40
CRUZADO, Kevin Tan	26	HIRORI, Hideki	56	KANEMITSU, Yoshihiko	56, 81
[D]		HIROSE, Hisaaki	20	KANNO, Natsuko	28
DENIS ROMERO, Fabio	66	HIROSE, Takashi	6, 80	KATO, Itsuki	54
[E]		HISATOMI, Ryusuke	18	KATO, Mariko	24
EBARA, Shunsuke	38	HONG, Yu Min	18	KATO, Tatsuhisa	14
ENDO, Hisashi	58, 82	HONJO, Kazuma	4	KAWAGUCHI, Yoshimasa	20
[F]		HOSOYO, Tomoki	12	KAWAKATSU, Hikaru	38
FANG, Tao	32	HOURLAI, Shinji	52	KAWAMOTO, Jun	34
FANG, Yue	58	HU, Shuai Feng	40, 82	KAWAMURA, Yuki	20
FARRAG, Asmaa Mostafa Abdelbari		HU, Weizhe	6	KAWARAZAKI, Ryo	18
Soliman	26	HUANG, Guanglin	6, 84	KAWASE, Riku	16
FU, Haining	16	[I]		KAWASHIMA, Hiroyuki	16
FUJIE, Masahiro	16	ICHIKAWA, Noriyo	52	KAYAHARA, Eiichi	14
FUJII, Tomomi	48	IDE, Shiina	58	KAZAMA, Hiroki	46
FUJIKAWA, Nana	6	IHOSHI, Makoto	52, 82	KIBUNE, Masato	14
FUJIMOTO, Seitarou	12	IJCHI, Wataru	4	KIHARA, Ayako	50
FUJIMURA, Kouki	8	IKEBUCHI, Tetsuya	18	KIJIMA, Soichiro	58
FUJISAKI, Yoshie	54	IKITOU, Asuka	20	KINOSE, Yuji	12
FUJIWARA, Masanori	16	IMAI, Makiko	50	KINOSHITA, Jun	40
FUKUMOTO, Koto	50	IMAMURA, Yuji	14	KISHI, Ryohei	76
FUNADA, Shinsaku	18	IMANISHI, Miki	20	KISHI, Shintaro	34
FUNASAKI, Tsukasa	40	IMAO, Keisuke	20	KISHIMOTO, Mizuki	36
FUTAKI, Shiroh	20, 80	IMURA, Naohiro	22	KITAYAMA, Kaori	34
[G]		INJAC, Sean	52	KITAYAMA, Yuki	50
GARCIA, Julius	4	INOUE, Hiromu	34, 81	KIYOMURA, Tsutomu	46
GARCIA, Kimberly Gacayon	58	INOUE, Tadashi	76	KOBAYASHI, Yuta	18
GO, Touran	50	ISERI, Kenta	50	KODAIRA, Satoshi	76
GOTO, Masato	52	ISHIDA, Takashi	76	KOMIYAMA, Haruka	18
GOTOH, Kana	14	ISHIDA, Toshiaki	22	KONDO, Yoshiko	76
GU, Jiajian	6	ISHIHARA, Kurauo	28	KOSUGI, Yoshihisa	52, 82
		ISHIHATA, Shota	36	KOYAMA, Ryota	12
		ISOBE, Kota	30	KUBOTA, Mikihiro	16
		ISODA, Yosuke	52	KURATA, Hiroki	46
		ISOZAKI, Katsuhiko	50	KURIHARA, Tatsuo	34
		ITOU, Yuuki	42	KURIYAMA, Masashi	20
		IWASAKI, Yasuko	40		

KUSAKABE, Yu	28	NAKAGAWA, Hiromichi	28	[R]	
KUWANO, Kyosuke	18	NAKAGAWA, Kotaro	56	REN, Yongxia	28
KUWATA, Mizuki	10	NAKAGAWA, Yuka	50	[S]	
KUWATA, Satoshi	36	NAKAGAWA, Yuna	20	SADAI, Shumpei	6
KUZE, Keita	42	NAKAJIMA, Atsushi	76	SAITO, Masahiro	12
[L]		NAKAJIMA, Yuki	12	SAITO, Ryohei	50
LAI, Ming Wei	46	NAKAMURA, Kaito	36	SAKAI, Takayuki	20
LI, Han	10	NAKAMURA, Masaharu	50	SAKAI, Yuta	54
LI, Ruiming	60	NAKAMURA, Tomoya	40	SAKAMOTO, Masanori	10
LI, Zhanzhao	10, 80	NAKAMURA, Yuki	50	SAKAMOTO, Minoru	56
LIN, Hao	10	NAKANISHI, Taiki	4	SAKAMOTO, Minoru	56
LIN, I-Ching	46	NAKANISHI, Yohei	36	SARUYAMA, Masaki	10
LIU, Chunting	60	NAKANISHI, Yohei	36	SASAYAMA, Ryuto	4
LIU, Wentao	40	NAKANO, Emiri	34	SATO, Hiroki	28
LIU, Wenwen	58	NAKANO, Shuichi	40	SATO, Hiroki	28
LIU, Zhibo	6	NAKASHIMA, Shogo	60	SATO, Ryota	10
LU, Siming	50	NAKATANI, Yuya	50	SATO, Shinichi	26
LU, Yangtian	14	NARITA, Hideki	18	SATO, Takeshi	38
[M]		NEMOTO, Takashi	46	SEKIGUCHI, Fumiya	56
MA, Yier	60	NGUYEN, Duc Anh	62	SEKIGUCHI, Yuhei	10
MACHI, Ryosuke	14	NGUYEN, Hao Canh	62	SEO, Haruna	12
MAEHARA, Yoshiki	42	NGUYEN, Thi Tuyen	58	SHEN, Yufan	10
MAENO, Ayaka	28	NISHIKAWA, Emina	62	SHIBAHARA, Keisuke	14
MAKINO, Momo	52	NISHIKAWA, Tetsuri	16	SHIH, Chi-Yu	58
MAMITSUKA, Hiroshi	62	NISHIO, Kosuke	26	SHIMAKAWA, Yuichi	52
MARU, Kousuke	14	NISHIYAMA, Hiroki	58	SHIMAZAKI, Ai	40
MASAKI, Asuka	34	NODA, Naotaka	26	SHIMOAKA, Takafumi	32
MASHIGUCHI, Kiyoshi	22	NOMURA, Satsuki	50	SHIOTA, Koji	60
MASUNO, Shin-ichiro	44	NOMURA, Yuki	36	SHIOTA, Yoichi	18, 80
MATSUDA, Hiroshi	50	NUKUI, Yousuke	12	SHIOYA, Nobutaka	32
MATSUKAWA, Kimihiro	12	[O]		SHIZU, Katsuyuki	28
MATSUKAWA, Tamaki	50	OGATA, Hiroyuki	58	SINGH, Vaibhav Pal	26
MATSUMIYA, Yumi	38	OGAWA, Hiroki	36	SODEOKA, Mikiko	76
MATSUMOTO, Kenshi	10	OGAWA, Takuya	34	SOHRIN, Yoshiki	30, 81
MATSUMURA, Hiroyuki	50	OGAWA, Tetsuya	46	SUGIURA, Itaru	18
MATSUOKA, Kohei	30	OGAWARA, Ryo	42	SUITO, Taisuke	4
MATSUOKA, Yuto	54	OHARA, Miu	38	SUWANAWAT, Nittikarn	34
MATSUSHIGE, Yuko	40	OHASHI, Noboru	40	SUZUKI, Katsuaki	28
MATSUSHITA, Shou	14	OHKI, Izuru	16	SUZUKI, Shogo	50
MENG, Lingjie	58	OHKI, Yasuhiro	54	[T]	
MICHIBATA, Junya	20	OHMI, Kyoko	28	TAHARA, Hirokazu	66, 82
MIYAJI, Kousuke	10	OHNO, Kohji	12	TAKAGI, Motoshige	60
MIYAKE, Yuya	6	OHTOMO, Masahiro	60	TAKAHATA, Ryo	10
MIZUHATA, Yoshiyuki	4	OKADA, Tasuku	12	TAKAMURA, Yoshiro	12
MIZUOCHI, Norikazu	16	OKANO, Syusuke	20	TAKANO, Shotaro	30
MORI, Takahiro	14	OKAZAKI, Yusuke	58	TAKAYA, Hikaru	50
MORI, Tomoya	60	OKUMURA, Kazuki	28	TAKEKUMA, Haruka	10
MORIKI, Yoshihito	12	OKUMURA, Ryosuke	28	TAKEMOTO, Kodai	22
MORIMOTO, Ryuji	36	OKUSHIMA, Ryota	6	TAKEMOTO, Misao	26
MORIOKA, Naoya	16	OMATSU, Yamato	80	TAKEMOTO, Yasushi	26
MORISHITA, Hiroki	16	ONO, Teruo	18	TAKEMURA, Yuki	16
MORISHITA, Taro	40	OTSUKI, Masashi	32	TAKENAKA, Mikihito	36
MORITA, Kouki	16	OSHIRO, Taku	4	TAKEWAKI, Yoshika	40
MORIYAMA, Takahiro	18	OTONARI, Kenko	20	TAMADA, Ric	34
MU, Lixuan	60	[P]		TAMAKI, Moeka	12
MURAMATSU, Tomomi	28	PASCUAL MIELGO, Jorge	40	TAMUKAI, Kento	20
MURATA, Yasujiro	6, 83	PERRON, Amelie	26	TAMURA, Takeyuki	60
MURDEY, Richard	40	PETSCHNER, Peter	62	TAN, Tiancheng	40
[N]		PINCELLA, Francesca	50	TANAKA, Hiroyuki	28
NAGAE, Ayumi	30	PRODINGER, Florian	58	TANAKA, Kamui	20
				TANIFUJI, Kazuki	54
				TANIGAKI, Yusuke	8
				TATSUYAMA, Tomomichi	30

TERANISHI, Toshiharu	10	YU, Coleman	60
TOH, Kohei	26	YUKIMOTO, Mariko	4
TOKITOH, Norihiro	4, 78	YUMOTO, Go	56
TOMITA, Kazutaka	32		
TONGU, Hiromu	42		
TOSAKA, Masatoshi	14	[Z]	
TRAN, Mai Chi	26	ZENG, Yuting	6
TRINH, Thang Thuy	10	ZHANG, Liwen	58
TRUONG, Minh Anh	40, 82	ZHANG, Ruixuan	58
TSERENDAGVA, Manchir	26	ZHANG, Sheng	6
TSUDZUKI, Taiku	34, 81	ZHANG, Yichen	14
TSUGE, Tomohiko	24	ZHANG, Zheng	6
TSUJI, Shingo	4	ZHANG, Zhenya	56
TSUJI, Takeshi	16	ZHAO, Hongda	58
TSUJII, Yoshinobu	12, 80	ZHENG, Chuyu	6
TSUKADA, Kyo	42	ZHENG, Leshang	14
TSURIBE, Hiroki	50	ZHENG, Linjie	30
		ZHU, Lingkai	10
		ZHU, Mengdi	58
[U]		ZHU, Mengshan	34
UCHIDA, Daichi	4	ZHU, Nanyi	14
UCHIDA, Gaku	16	ZHU, Xiaotan	6
UEBERRICKE, Lucas Veith	40		
UEDA, Kunihiro	85		
UEDA, Yoshihiro	8, 80		
UEKI, Ryuta	30		
UESUGI, Motonari	26		
[W]			
WAKAMIYA, Atsushi	40, 81		
WAKASUGI, Masanori	42		
WAKIOKA, Masayuki	54		
WANG, Feiqi	60		
WATANABE, Bunta	22		
WATANABE, Hiroshi	38, 79		
WATANABE, Rei	52		
WATANABE, Yuki	36		
WATARI, Machiko	24		
WU, Beiling	50		
WU, Jia-De	14		
WU, Junyi	58		
[X]			
XIA, Jun	58		
XIE, Lingling	52		
[Y]			
YABUUCHI, Naoaki	76		
YAMADA, Kohei	58		
YAMADA, Takumi	56		
YAMAGO, Shigeru	14		
YAMAGUCHI, Atsushi	46		
YAMAGUCHI, Shinjiro	22		
YAMAMOTO, Tomokazu	58		
YAMAUCHI, Taisei	16		
YANADA, Mizuho	12		
YANG, Qingwei	58		
YANG, Yi	4		
YAO, Hajime	16		
YASUDA, Keiko	24		
YIN, Haozhi	50		
YOSHIDA, Mariko	32		
YOSHIDA, Sayuri	22		
YOSHIE, Shunsuke	20		

KEYWORD INDEX

[A]		[H]		[P]	
Accelerator Physics	42	Helical Structures	6	Peptide Design	20
Amorphous Materials	28	Heteroatom	4	Perfluoroalkyl Compounds	32
Analytical Chemistry	30	Heterointerface	52	Perovskite Solar Cells	40
		Hierarchical Structure	36	Perovskites	56
[B]		High Harmonic Generation	56	Phospholipid Acyltransferase	34
Bacterial Cold-adaptation Mechanism	34	High Pressure Synthesis	52	Phospholipid Signaling	24
Beam Physics	42	Homogeneous Catalysis	54	Photocatalysts	10
Bioinformatics	58, 62	Hybrid Materials	12	Plant Hormone	22
Bioinorganic Chemistry	54			Plasmonics	10
Biosynthesis	22	[I]		pMAIRS and MAIRS2	32
Boolean Networks	60	Immunology	26	Polymer Brush	12
		Infrared and Raman Spectroscopy	32	Polymer Physics	36
[C]		Inorganic Nanoparticles	10	Polymer Properties	14, 36
Chemical Biology	26	Intense Laser Science	44	Polymer Synthesis	14
Chemical Genetics	26	Intracellular Delivery	20	Polyunsaturated Fatty Acid	34
Chemical Graphs	60	Iron Catalysis	50	Precision Polymerization	12
Chemical Library	26			Protein Crystallography	48
Complex Networks	60	[K]		Protein Informatics	60
Computational Genomics	62	Kinetic Stabilization	4		
π -Conjugated Systems	6			[Q]	
COP9 Signalosome	24	[L]		Quantum Chemical Calculation	28
Core-Hole	46	Laser Nano-Ablation Physics	44	Quantum Information Science	16
Crystal	48	Laser Plasma Radiations (Electrons, Ions, and THz)	44	Quantum Materials	16
Curved π -Conjugated Molecules	14	Living Radical Polymerization	12, 14	Quantum Sensing	16
Cytochrome P450	22	Low-Coordinated Species	4		
				[R]	
[D]		[M]		Radical Species	6
Data Mining	62	Machine Learning	62	Receptor	22
Diamond	16	Magnetic Materials	18	Rheology	38
Dielectric Spectroscopy	38	Magnetism	18	RNA	24
DNA/RNA Binding Protein	20	Marine Chemistry	30		
Dynamic Nuclear Polarization Enhanced NMR	28	Membrane Curvature	20	[S]	
		Membrane-Permeable Peptides	20	Self Assembly	36
[E]		Metal Ion Recognition	30	Semiconductor Nanoparticles	56
EELS	46	Metal Nanocluster	50	Semiconductors	40
ELNES	46	Molecular Aggregation	40	Signal Transduction	24
Endohedral Fullerenes	6	Molecular Catalyst	8	Single Electronics	10
Environmental Genomics	58	Molecular Design and Synthesis	40	Single Photon Spectroscopy	56
Epitaxial Thin Film Growth	52	Molecular Evolution	58	Site-Selective Functionalization	8
Extracellular Membrane Vesicle	34	Molecular Recognition	8	Small Molecules	26
Extremophiles	34	Morphogenesis	24	Softmatter	36, 38
				Solid State Chemistry	52
[F]		[N]		Solid-State NMR	28
Femtosecond Laser Processing	44	Nanocomposite Magnet	10	Spintronics	18
Femtosecond Laser Spectroscopy	56	Natural Product	8	Stable Isotopes	30
First-Principle Calculation	46	Neural Networks	60	STEM	46
Functional Materials	6, 40	Neutron Optics	42	Steric Protection	4
Functional Metal Oxides	52	Nitrogen Fixation	54	Storage Ring	42
		NV Center	16	Strigolactone	22
[G]				Structural Biology	48
GenomeNet	58	[O]		Structure and Function	48
		Organic Light-Emitting Diodes	28	Sugar	8
		Organic Semiconductors	32	Supramolecular Catalysis	50
		Organic Synthesis	14	Surface and Interface Chemistry	32
				Synthetic Organic Chemistry	50

Systems Biology	62
[T]	
Trace Elements	30
Transition Metal Clusters	54
Transition Metal Complexes	4
Tribology	12
[U]	
Ultrafast Electron Diffraction (UED)	44
Unstable Nuclear Physics	42
[V]	
Virology	58
[W]	
Woody Biomass	50
[X]	
X-ray Crystallographic Analysis	48

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R_esearch

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