Pioneering Project
Research Activity Report
新領域開拓課題 研究業績報告書

Fundamental Principles Underlying the Hierarchy of Matter
物質階層原理
Lead Researcher: Reizo KATO
研究代表者：加藤 礼三
From April 2017 to March 2020

Heterogeneity at Materials Interfaces
ヘテロ界面
Lead Researcher: Yousoo Kim
研究代表者：金 有洙
From April 2018 to March 2020

RIKEN May 2020

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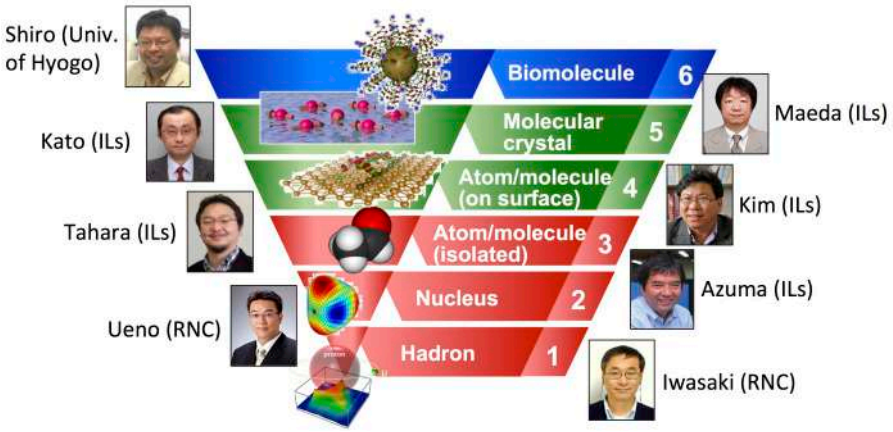
Outline

（１）「物質階層原理」と「ヘテロ界面」の概要 / Outline of two projects

Fundamental Principles Underlying the Hierarchy of Matter: A Comprehensive Experimental Study / 物質階層原理

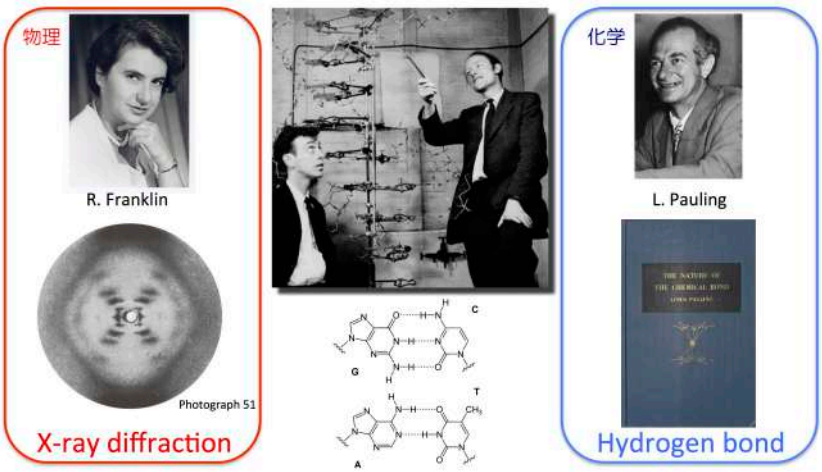
• *Outline of the Project*

This five-year project lead by Dr. R. Kato is the collaborative effort of eight laboratories, in which we treat the hierarchy of matter from hadrons to biomolecules with three underlying and interconnected key concepts: *interaction*, *excitation*, and *heterogeneity*. The project consists of experimental research conducted using cutting-edge technologies, including lasers, signal processing and data acquisition, and particle beams at RIKEN RI Beam Factory (RIBF) and RIKEN Rutherford Appleton Laboratory (RAL).



• *Physical and chemical views of matter lead to major discoveries*

Although this project is based on the physics and chemistry of non-living systems, we constantly keep all types of matter, including living matter, in our mind. The importance of analyzing matter from physical and chemical points of view was demonstrated in the case of DNA. The Watson-Crick model of DNA was developed based on the X-ray diffraction, which is a physical measurement. The key feature of this model is the hydrogen bonding that occurs between DNA base pairs. Watson and Crick learned about hydrogen bonding in the renowned book “The Nature of the Chemical Bond,” written by their competitor, L. Pauling, who was a leading authority on chemical bonding. This important lesson in history teaches us that viewing matter from physical and chemical perspectives can lead to dramatic advances in science.



• *Hierarchy of Matter: Universality vs. Diversity*

We believe that the behavior of matter, including biological systems, can be understood through physical laws. P. Dirac, a great physicist, stated this universality as follows: "once we know the underlying physical laws*, the rest is chemistry*." On the other hand, P. W. Anderson, another great physicist, claimed that the interactions among multiple components in complex systems create entirely new properties in each layer of the hierarchy, with his famous phrase "*More is different*". This means that the science governing each layer is different, and it is not until we understand this diversity that we understand the universal principles completely. Therefore, we have selected "interaction" as the first key concept of this project. In addition, we selected "excitation" and "heterogeneity" as the other important key concepts to understand diversity in the hierarchy.

普遍性

P. Dirac

• *The rest is chemistry*

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

The behavior of matter including biological systems can be understood through physical laws.

多様性

P. W. Anderson

• *More is different*

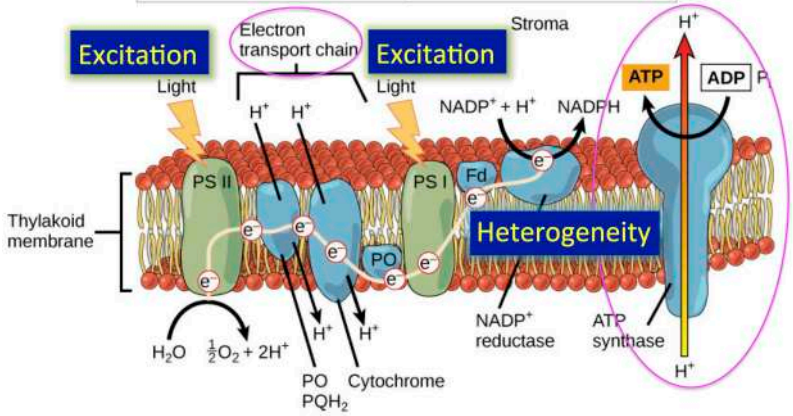
The behavior of large and complex aggregates of elementary particles is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear.

The interactions among multiple components in complex systems create entirely new properties in each layer of the hierarchy.

• *Three Key Concepts: Interaction, Excitation, and Heterogeneity*

The importance of these three key concepts is well illustrated by the photochemical reaction system, involved in photosynthesis. First, the photosynthesis proceeds in the thylakoid membrane, which has a heterogeneous structure. This *heterogeneity* is essential for the emergence of the functionality of the membrane. *Excitation* by light is the most important step in photosynthesis. Finally, important processes, including electron transport and ATP synthesis, are controlled by various *interactions*.

Photochemical reaction system（光合成の明反応）

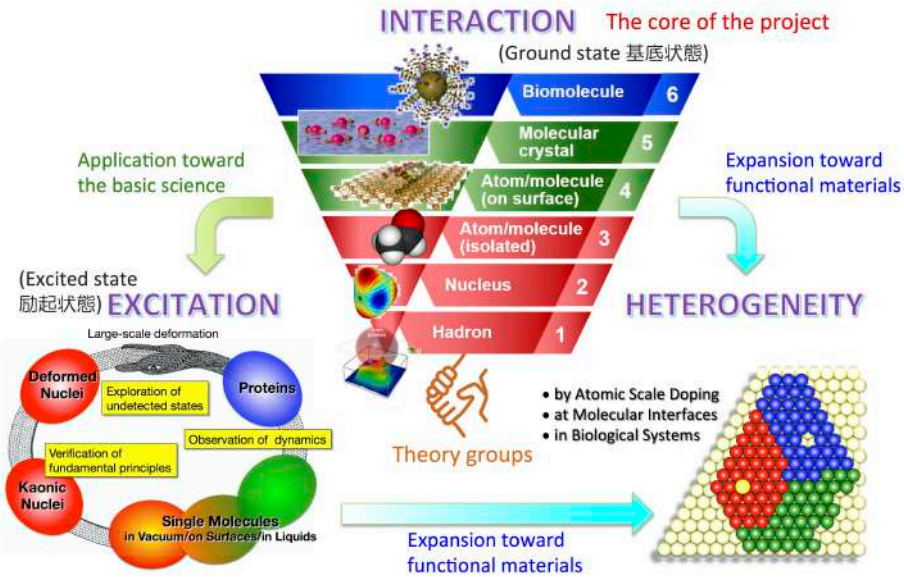


Important functions, including electron transport and ATP synthesis, are controlled by various INTERACTIONs

• *Three Key Concepts and Sub-projects*

The three key concepts are associated with three sub-projects: "Interaction in matter" lead by Dr. Ueno,

"Excitation in matter" lead by Dr. Azuma, and "Heterogeneity in matter" lead by Dr. Kim. As mentioned, the "Interaction" sub-project is the core of this project. To comprehensively understand the nature of interactions that take place in each layer, it is essential to collaborate with theory groups. The knowledge obtained by the "Interaction" sub-group will be applied toward the basic science of excitation. The "Interaction" sub-project investigates the ground state of systems, and the "Excitation" sub-project focuses on the excited states of systems. The results obtained by these two sub-projects will be expanded towards the development of functional materials by the "Heterogeneity" sub-group. A unique point of this project is that almost all members participate in more than two sub-projects, which enhances comprehensive understanding of these concepts.



• *Interaction in Matter*

The "Interaction" sub-group investigates the diversity of phenomena caused by interactions that occur in each level in the hierarchy of matter. The strong interaction and the electromagnetic interaction give rise to a variety of phenomena depending on many-body effects, geometry, dimensionality, external conditions and so on. The interactions studied by each team range from the strong interaction between quarks to the van der Waals interaction between single-stranded DNA molecules, with a focus on how interactions in systems with multiple degrees of freedom lead to a diversity of phenomena. This means that many-body effects and multiple degrees of freedom are key issues in every layer of the hierarchy.

• *Excitation in Matter*

Excitation is a key step for the emergence of functionality, but knowledge on this topic is surprisingly limited. Thus, in this sub-group, we carry out three types of research on excitation, "Exploration of undetected excited states" in deformed nuclei, "Verification of fundamental principles through excited states" in kaonic nuclei, and "Observation of excited state dynamics" in excited molecules in liquids, on surfaces, and in vacuum. We study excitation over a wide range of energies, sizes, and time scales. At the same time, we study universality as indicated by the large-scale deformations observed in both excited-state nuclei and proteins.

• *Heterogeneity in Matter*

Heterogeneity is an important spatial property for the emergence of functionality as well as a challenging research target that drives the development of cutting-edge measurement technologies. This sub-group will apply the results of the "Interaction" and "Excitation" sub-groups toward the development of functional materials. In this sense, the "Heterogeneity" sub-group is closely tied to practical applications. The main topics investigated are superconducting doped diamond (as "Heterogeneity by Atomic Scale Doping"),

electrical double layers in the field effect transistors (as “Heterogeneity at Molecular Interfaces”), and lipid membranes in solution (as “Heterogeneity in Biological Systems”), which are tackled through a wide range of collaborations.

• *Goal of the Project*

The most important goal of the project is the construction of a new cross-disciplinary research network based on the bottom-up style research activities at RIKEN, which will drive a dramatic evolution of science and lead to unpredictable by-products. This network includes *ExpRes Dojo* where we share, learn, and report information on cutting-edge experimental technologies, primarily laser and signal processing and data acquisition technologies. This consists of school-type meetings and workshops. An important output of the *ExpRes Dojo* is the application of new technologies developed thorough the physics and chemistry research to biological systems. At the same time, we nurture young researchers with wider and deeper views of matter. We believe that the scientific community is one where innovative discoveries are frequently achieved by newcomers in different research fields. The present project will maintain the diversity of science at RIKEN and ensure an environment in which young researchers with high ambitions can easily cross over the boundaries between disciplines.

Heterogeneity at Materials Interfaces / ヘテロ界面

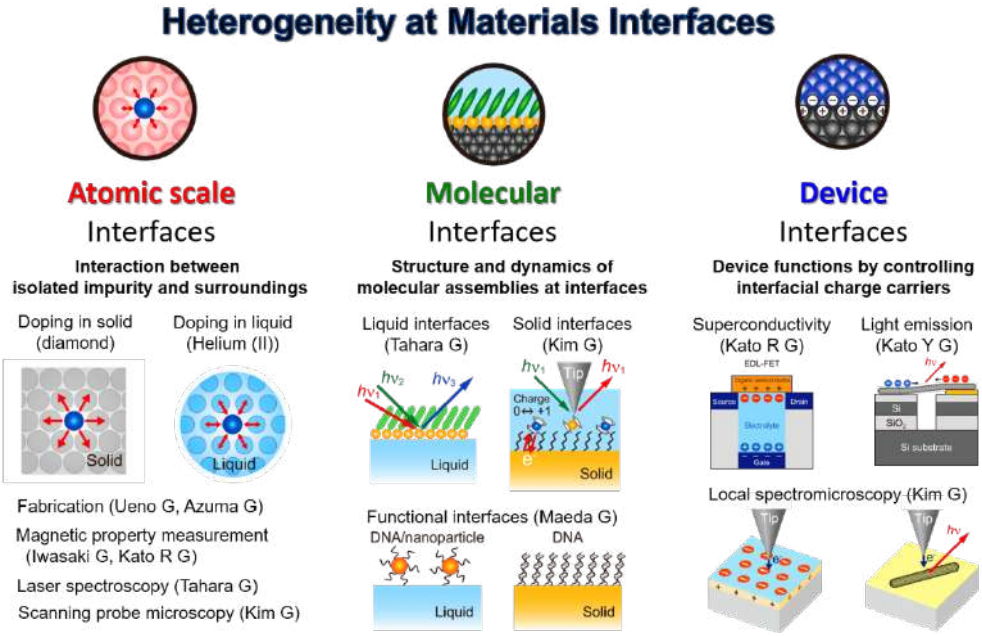
• *Reorganization of the Project*

The proposal “Fundamental Principles Underlying the Hierarchy of Matter: A Comprehensive Experimental Study”「物質階層原理」(Lead Researcher: Dr. R. Kato) was highly evaluated and launched in 2017. Unfortunately, however, the budget was heavily reduced and thus we had to start the project with “Interaction” and “Excitation” subgroups in the reduced form and removed the “Heterogeneity” group. In order to recover the original purpose, we proposed a new five-year pioneering project “Heterogeneity at Materials Interfaces” 「ヘテロ界面」lead by Dr. Y. Kim. This new proposal was also highly evaluated and launched in 2018. As a result, we have realized the original proposal in the form of two pioneering projects. Because they share the same scientific concept, they are managed in association with each other.

• *Outline of the Project*

The heterogeneity at the interface between two different materials plays pivotal roles in transport of charge, matter, and energy across the interfaces, chemical reactions and interactions, functions of materials and devices, and biological activities in living systems. However, it is still far from the detailed description of them mainly due to the structural and phenomenal complexity at the interfaces. It is, thus, a great scientific challenge to investigate the heterogeneity at interfaces, and it eventually appears to be of profound importance for our future society to understand the processes occurring at the interfaces and to make wise and practical use of them. This project aims at understanding and controlling structures and functions originated in heterogeneity at a variety of interfaces that encompass (A) interaction of a single dopant with surroundings in solid and liquid materials, (B) structures, functions and reactions of molecular interfaces and (C) development of new functional devices by controlling interface charge carries, by corresponding three sub-projects. Scientists of world-leading laboratories (Chief Scientist Laboratories) and a top-level research infrastructure (Nishina Center for Accelerator-Based Science) in RIKEN put together their research competences to accomplish the mission. Total of eight research groups participating in this project cover a wide range of research fields such as physics, chemistry, biotechnology, and engineering. This project is also characterized by its novel organization where the various research fields are intertwined in each sub-project, which provides a large synergistic effect.質We also tackle fundamental scientific issues closely related to the functional expression of interfaces in materials systems in a complementary way with other pioneering

project, “Fundamental Principles Underlying the Hierarchy of Matter: A Comprehensive Experimental Study”. All these activities will enable us to develop cutting-edge measurement and device technology, to apply the discovered functions to practical use, and to nurture young researchers with the skills and abilities required to ensure the future success in the field of materials science.



• *Sub-projects and Missions*

(A) Heterogeneity at atomic-scale interface (lead by Dr. Ueno)

At atomic-scale interfaces, isolated impurities are introduced to solid (single-crystal diamond) and to liquid (He II) to understand the quantum-level interactions between each dopant with surrounding atoms. We challenge to realize superconducting diamond by high-concentration doping of nitrogen (n-type) for the first time, although superconductivity of boron-doped (p-type) diamond has been reported. It is still unknown how the quantum interaction occurs among the dopants and surrounding atoms to evolve unprecedent phenomena, which is a crucial issue to understand and utilize heterogeneity at atomic-scale interfaces in matters.

(B) Heterogeneity at molecular interface (lead by Dr. Tahara)

At molecular interfaces, our knowledge and ability to control the molecular interfaces at the molecular-level are very immature, compared to those for the molecules in the bulk, although the molecular interfaces play essential roles in various phenomena such as wetting, adhesion, biocompatibility, tribology, electrical properties as well as complex reactions in living things. Therefore, a concerted spectroscopic and microscopic study is highly desired for elucidating structural and functions of molecular interfaces.

(C) Heterogeneity at device interface (lead by Dr. Kim)

At device interfaces, the heterogeneity of electric field at the electrode interface largely influences on the various kinds of charge carrier dynamics, such as electron/hole injection, trapping, recombination and transport, which play a central role in device performance. We will evolve novel functions of organic transistor devices, such as superconductivity and light emission, by controlling charge carriers at the interface between electrodes and materials, based on the atomic/molecular-level understanding of charge carrier distribution and dynamics at the device interface.

（２）研究体制 / Research System

Eight groups in RIKEN (from CPR and RNC) join two projects. In addition, we are in collaboration with four research groups outside RIKEN (from Univ. of Hyogo, TIT, IMS, and Osaka Univ.). Almost all members participate in more than two sub-projects that are classified by the research category number in this activity report as follows:

	物質階層原理		ヘテロ界面		
Category	**1**	**2**	**3**	**4**	**5**
M. Iwasaki	○	○	○		
H. Ueno	◎	○	◎		
T. Azuma	○	◎	○		
Y. Kim	○	○	○	○	◎
R. Kato	○		○		○
T. Tahara		○	○	◎	
M. Maeda	○			○	
Y. Kato					○
Y. Shiro*	○	○		○	
M. Fujii*	○				
H. Yamamoto*					○
H. Noumi*		○			

* outside RIKEN質質◎ Sub-project leader

	Research category (Sub-group)
物質階層原理	1. Interaction in matter
	2. Excitation in matter
ヘテロ界面	3. Atomic-scale interfaces
	4. Molecular interfaces
	5. Device interfaces

（３）代表的な研究成果 / Major research achievements (Research Category in [ ])

物質階層原理

1. "$K^{-}pp$", a K-meson nuclear bound state, observed in ^{3}He(K^{-}, Λp)n reactions [1]
（^{3}He(K^{-}, Λp)n 反応による K 中間子束縛原子核状態 "$K^{-}pp$" の発見）
M. Iwasaki, T. Yamaga, F. Sakuma, H. Noumi, Y. Ma, H. Asano, and for the J-PARC E15 Collaboration, Phys. Let. B, **789**, 620 (2019)

2. RICE: Riken Cryogenic Electrostatic ion storage ring [1,2]
（RICE:理研極低温静電型イオン蓄積リング）
Y. Nakano, Y. Enomoto, T. Masunaga, S. Menk, P. Bertier and T. Azuma,
Rev. Sci. Instrum. **88**, 033110 (2017)

3. Temporal Mapping of Electrophilic Photochemical Reactions and Excitonic Processes with Carbon Specificity [1]
（求電的な光化学反応と炭素特異性のある励起過程の時間分解）
K. Wang, P. Murahari, K. Yokoyama, J.S. Lord, F.L. Pratt, J. He, L Schulz, M Willis, J.E. Anthony, N.A. Morley, L. Nuccio, A. Misquitta, D.J. Dunstan, K. Shimomura, I. Watanabe, S Zhang, P. Heathcote, and A.J. Drew, Nature Materials **16**, 467–473 (2017).

4. Atomic-scale visualization of the stepwise cycloaddition reaction pathways by intermolecular interaction on a metal surface [1, 4]
（金属表面上における分子間相互作用による環化付加反応経路の可視化）
C. Zhang, E. Kazuma, and Y. Kim, Angew. Chem. Int. Ed., **58**, 17736-17744 (2019)

5. Discovery of on-surface evolution of meso-isomerism in 2D supramolecular assemblies [1, 4]
（二次元超分子集合体におけるメソ異性の表面進化の発見）
J. Park, J.-H. Kim, S. Bak, K. Tahara, J. Jung, M. Kawai, Y. Tobe, and Y. Kim,
Angew. Chem. Int. Ed., **58**, 9611-9618 (2019).

6. Synthesis of centimeter-scale and highly crystalline 2D alcohol at a graphene [1, 4]
（グラフェンにおけるセンチメートルスケールで高結晶性を有する二次元アルコールの合成）
H. Lim, Y. Park, M. Lee, J.-G. Ahn, B.-W. Li, Da Luo, J. Jung, R. Ruoff, and Y. Kim, Nano Lett., **20**, 2107-2112 (2020).

7. Discovery of the Dirac electron system in a single-component molecular conductor [1]
（単一成分分子性導体におけるディラック電子系の発見）

R. Kato, H. B. Cui, T. Tsumuraya, T. Miyazaki, and Y. Suzumura, J. Am. Chem. Soc., **139**, 1770 (2017)

8. Discovery of an interplay between spin, charge, lattice and orbital in molecular quantum spin liquid [1]
（分子性量子スピン液体におけるスピン・電荷・格子・軌道の連動性の解明）
T. Yamamoto, T. Fujimoto, T. Naito, Y. Nakazawa, M. Tamura, K. Yakushi, Y. Ikemoto, T. Moriwaki, and R. Kato, Scientific Reports, **7**, 12930 (2017)

9. Discovery of intramolecular fragmentation of magnetic moments near quantum spin liquid [1]
（量子スピン液体相近傍での磁気モーメントの分子内分裂の発見）
S. Fujiyama and R. Kato, Phys. Rev. Lett., **122**, 147204 (2019)

10. Molecular Recognition by a Short Partial Peptide of the Adrenergic Receptor: A Bottom-Up Approach [1, 4]
（アドレナリン受容体の短い部分ペプチドによる分子認識：ボトムアップアプローチ）
T. Sekiguchi, M. Tamura, H. Oba, P. Çarçarbal, R. R. Lozada-Garcia, A. Zehnacker-Rentien, G. Grégoire, S. Ishiuchi, M. Fujii, Angew. Chem. Int. Ed. **57**, 5626 (2018). (**Journal Cover**) [1,4]

11. Can the Partial Peptide SIVSF of the β_2-Adrenergic Receptor Recognize Chirality of the Epinephrine Neurotransmitter? [1, 4]
（β_2—アドレナリン受容体の部分ペプチド SIVSF はアドレナリン（エピネフリン）のキラリティを認識するか）
M. Tamura, T. Sekiguchi, S. Ishiuchi, A. Zehnacker-Rentien, M. Fujii, J. Phys. Chem. Lett. **10**, 2470 (2019). (**Journal Cover**)

12. Alkali and alkaline earth metal ions complexes with a partial peptide of the selectivity filter in K^+ channels studied by a cold ion trap infrared spectroscopy [1, 4]
（冷却イオントラップ赤外分光法によるアルカリ金属およびアルカリ土類金属とカリウムイオンチャネル選択フィルターの部分ペプチドとの錯体の研究）
R. Otsuka, K. Hirata, Y. Sasaki, J. M. Lisy, S. Ishiuchi, M. Fujii, ChemPhysChem in press, DOI: 10.1002/cphc.202000033 (**Journal Cover**)

13. Interaction of Proteins with Other Molecules Regulates Biological Functions: Nitric Oxide Reductase [1]
（タンパク質相互作用による生理的機能の制御：脱窒系酵素群）
E. Terasaka, K. Yamada, P.-H. Wang, K. Hosokawa, R. Yamagiwa, K. Matsumoto, S. Ishii, T. Mori, K. Yagi, H. Sawai, H. Arai, H. Sugimoto, Y. Sugita, Y. Shiro, T. Tosha
Proc. Natl. Acad. Sci. USA **114**, 9888-9893 (2017)

14. Interaction of Proteins with Other Molecules Regulates Biological Functions: Oxygen Sensor System [1]

（タンパク質相互作用による生理的機能の制御：酸素センサーシステム）
G. S. A. Wright, A. Saeki, T. Hikima, Y. Nishizono, T. Hisano, M. Kamaya, K. Nukina, H. Nishitani, H. Nakamura, M. Yamamoto, S. V. Antonyuk, S. S. Hasnain, Y. Shiro, H. Sawai
Sci. Signal. **11**, aaq0825 (2018)

15. Development of a method for directed assembly of nanoparticles with an anisotropic structure [1]
（構造異方性ナノ粒子集合体の配向制御法の開発）
G. Wang, Y. Akiyama, N. Kanayama, T. Takarada, and M. Maeda, Small, **13**, 1702137 (2017)

16. Development of a method for folding nanoparticle chains into two-dimensional arrays [1]
（ナノ粒子鎖状集合体の折りたたみによる２次元アレイ構築法の開発）
S. Shiraishi, L. Yu, Y. Akiyama, G. Wang, T. Kikitsu, K. Miyamura, T. Takarada, and M. Maeda, Adv. Mater. Interfaces, **5**, 1800189 (2018)

17. Development of a method for directed assembly of isotropic nanoparticle oligomers [1]
（構造等方性ナノ粒子集合体の配向制御法の開発）
L. Yu, S. Shiraishi, G. Wang, Y. Akiyama, T. Takarada, and M. Maeda, J. Phys. Chem. C, **123**, 15293 (2019)

18. Development of a method for measuring interfacial forces emerging between brush-like DNA layers [1]
（DNA ブラシ層間に発現する界面力の測定法の開発）
T. Sekine, N. Kanayama, K. Ozasa, T. Nyu, T. Hayashi, and M. Maeda, Langmuir, **34**, 15078 (2018)

19. Phototaxis and photo-shock responses of Euglena gracilis under gravitaxis [1]
（重力走性下でのユーグレナの光走性と光ショック応答）
K. Ozasa, J. Won, S. Song, T. Shinomura, and M. Maeda, Algal Res., **41** 101563 (2019)

20. Carotenoids are essential for light perception by the eyespot apparatus to initiate the phototactic movement of Euglena gracilis [1]
（ユーグレナの光走性の始動には眼点のカロテノイドが必須である）
S. Kato, K. Ozasa, M. Maeda, Y. Tanno, S. Tamaki, M. Higuchi-Takeuchi, K. Numata, Y. Kodama, M. Sato, K. Toyooka, and T. Shinomura, Plant J., **101** 1091-1102 (2020)

21. Measurement of the magnetic moment of ^{75}Cu reveals the interplay between nuclear shell evolution and shape deformation [2]
（^{75}Cu の励起状態の核磁気モーメント測定で探る殻構造と変形の相互影響）
Y. Ichikawa, H. Nishibata, Y. Tsunoda, A. Takamine, K. Imamura, T. Fujita, T. Sato, S. Momiyama, Y. Shimizu, D. S. Ahn, K. Asahi, H. Baba, D. L. Balabanski, F. Boulay, J. M. Daugas, T. Egami, N. Fukuda, C. Funayama, T. Furukawa, G. Georgiev, A. Gladkov, N. Inabe, Y. Ishibashi, Y. Kobayashi, S. Kojima, A. Kusoglu, T. Kawaguchi, T. Kawamura, I. Mukul, M. Niikura, T. Nishizaka, A. Odahara, Y.

Ohtomo, T. Otsuka, D. Ralet, G. S. Simpson, T. Sumikama, H. Suzuki, H. Takeda, L. C. Tao, Y. Togano, D. Tomonaga, H. Ueno, H. Yamazaki and X. F. Yang, Nat. Phys. **15**, 321–325 (2019).

22. *g*-Factor of the ^{99}Zr (7/2^{+}) isomer: Monopole evolution in shape coexisting region [2]
（^{99}Zr の準安定励起準の *g* 因子測定で探る変形共存する核質量領域での単極子相互作用）
F. Boulay, G. S. Simpson, Y. Ichikawa, S. Kisyov, D. Bucurescu, A. Takamine, D. S. Ahn K. Asahi, H. Baba D. L. Balabanski, T. Egami, T. Fujita, N. Fukuda C. Funayama, T. Furukawa, G. Georgiev, A. Gladkov, M. Hass, K. Imamura, N. Inabe Y. Ishibashi, T. Kawaguchi, T. Kawamura, W. Kim, Y. Kobayashi, S. Kojima, A. Kusoglu, R. Lozeva, S. Momiyama, I. Mukul, M. Niikura, H. Nishibata, T. Nishizaka, A. Odahara, Y. Ohtomo, D. Ralet, T. Sato, Y. Shimizu T. Sumikama H. Suzuki H. Takeda L. C. Tao, Y. Togano, D. Tominaga, H. Ueno, H. Yamazaki, X. F. Yang, J. M. Daugas, Phys. Rev. Lett. **124**, 112501 (2020).

23. Radiative cooling dynamics of isolated N_2O^+ ions in a cryogenic electrostatic ion storage ring [2]
（極低温静電型イオン蓄積リング中の孤立 N_2O^+の放射冷却ダイナミクス）
A. Hirota, R. Igosawa, N. Kimura, S. Kuma, K. C. Chartkunchand, P. M. Mishra, M. Lindley, T. Yamaguchi, Y. Nakano and T. Azuma,
Phys. Rev. A. *submitted*.

24. Tracking photoinduced Au-Au bond formation through transient terahertz vibrations observed by femtosecond time-domain Raman spectroscopy [2]
（フェムト秒時間領域ラマン分光で観測される過渡的テラヘルツ振動による光誘起金-金結合生成の追跡）
H. Kuramochi, S. Takeuchi, M. Iwamura, K. Nozaki and T. Tahara, J. Am. Chem. Soc., **141**, 19296 (2019).

25. Microsecond conformational dynamics of biopolymers revealed by dynamic-quenching two-dimensional fluorescence lifetime correlation spectroscopy with single dye-labeling [2]
（動的消光二次元蛍光寿命相関分光によって明らかにされた生体高分子のマイクロ秒コンフォメーションダイナミクス）
B. Sarkar, K. Ishii and T. Tahara, J. Phys. Chem. Lett., **10**, 5536-5541 (2019).

26. Probing the early stages of photoreception in photoactive yellow protein with ultrafast time-domain Raman spectroscopy [2]
（超高速時間時間領域分光による光活動性黄色蛋白質の光受容初期段階の観測）
H. Kuramochi, S. Takeuchi, K. Yonezawa, H. Kamikubo, M. Kataoka and T. Tahara, Nat. Chem., **9**, 660- 666 (2017).

27. Development of single-molecule absorption spectroscopy with STM [2]
（STM を用いた単分子吸収分光法の開発）

H. Imada, K. Miwa, M. Imai-Imada, S. Kawahara, K. Kimura, and Y. Kim, Phys. Rev. Lett., **119**, 013901, 1-6 (2017).

28. Realization of a direct pathway to molecular photodissociation on metal surfaces using visible light [2]
（可視光による金属表面での分子光解離への直接経路の実現）
E. Kazuma, J. Jung, H. Ueba, M. Trenary, and Y. Kim, J. Am. Chem. Soc., **139**, 3115-3121 (2017)

29. Real-space and real-time observation of a plasmon-induced chemical reaction of a single molecule [2,4]
（単一分子におけるプラズモン誘起化学反応の実空間および実時間観察）
E. Kazuma, J. Jung, H. Ueba, M. Trenary, and Y. Kim, Science, **360**, 521-526 (2018)

30. Dynamics of Nitric Oxide in Biological System Examined using Excitation of Caged NO [2]
（ケージド NO の光励起を活用した、生体内 NO の動態解析：脱窒菌一酸化窒素還元酵素）
H. Takeda, T. Kimura, T. Nomura, A. Yokota, A. Matsubayashi, S. Ishii, T. Tosha, Y. Shiro, M. Kubo Bull. Chem. Soc. Japan (2020) *in press*

31. Dynamics of Nitric Oxide in Biological System Examined using Excitation of Caged NO [2]
（ケージド NO の光励起を活用した、生体内 NO の動態解析：脱窒カビ一酸化窒素還元酵素）
T. Tosha, et al. Nat. Commun. **8**, 1585 (2017)

32. Structure of charmed Baryons studied by pionic decays [2,1]
(π 崩壊で調べるチャームバリオンの構造)
H. Nagahiro, S. Yasui, A. Hosaka, M. Oka, and H. Noumi, Phys. Rev. **D95**, 014023(2017)

33. Experimental Investigation for Diquark Degrees of Freedom in a Charmed Baryon at J-PARC [2,1]
（J-PARC におけるチャームバリオン中のダイクォーク自由度の実験研究）
T.N. Takahashi for the J-PARC E50 collaboration, JPS Conf. Proc. **13**, 020042(2017)

34. Physics in J-PARC Hadron-Hall Extension [2,1]
(J-PARC ハドロンホール拡張における物理)
H. Noumi, JPS Conf. Proc. **13**, 010017(2017)

35. Strange and Charm Hadron Physics at J-PARC in Future [2,1]
（将来の J-PARC におけるストレンジとチャームハドロン物理)
H. Noumi, JPS Conf. Proc. **17**, 111003(2017)

36. Experimental Study of Di-quark Correlation by Charmed Baryon Spectroscopy at J-PARC High-Momentum Secondary Beam Line [2,1]
（J-PARC 高運動量二次ビームラインにおけるチャームバリオン分光によるダイクォーク相関

の実験研究）
Y. Komatsu et al., JPS Conf. Proc. **26**, 022029 (2019).

ヘテロ界面

1. Absolute optical absorption cross-section measurement of Rb atoms injected into superfluid helium using energetic ion beams [3, 2]
（超流動ヘリウム中に導入された高エネルギーRb 原子の光吸収反応断面積）
K. Imamura, Y. Matsuo, W. Kobayashi, T. Egami, M. Sanjo, A. Takamine, T. Fujita, D. Tominaga, Y. Nakamura, T. Furukawa , T. Wakui , Y. Ichikawa, H. Nishibata, T. Sato, A. Gladkov, L. C. Tao, T. Kawaguchi, Y. Baba , M. Iijima , H. Gonda , Y. Takeuchi , R. Nakazato , H. Odashima , and H. Ueno, App. Phys. Exp. **12**, 016502 (2019).

2. Impact of a hydrophobic molecular ion in the early stage of cloud formation [3]
（雲生成初期段階における疎水性分子イオンの影響）
L. Feketeová, P. Bertier, T. Salbaing, T. Azuma, F. Calvo, B. Farizon, M. Farizon, and T. D. Märk, PNAS **116**, 22540-22544 (2019).

3. Quadrupole mechanism for vibrational sum frequency generation at air/liquid interfaces: Theory and experiment [4]
（空気／液体界面における振動和周波発生の四重極機構：理論と実験）
K. Matsuzaki, S. Nihonyanagi, S. Yamaguchi, T. Nagata, and T. Tahara, J. Chem. Phys., **151**, 064701 (2019).

4. The topmost water structure at a charged silica/aqueous interface revealed by heterodyne-detected vibrational sum frequency generation spectroscopy [4]
（ヘテロダイン検出振動和周波分光で明らかになった帯電したシリカ／水溶液界面最上層の水構造）
S. Urashima, A. Myalitsin, S. Nihonyanagi, and T. Tahara: J. Phys. Chem. Lett., **9**, 4109-4114 (2018).

5. Probing structural changes in electrochemically active self-assembled monolayers [4]
（電気化学的活性を持つ自己組織化単分子層の構造変化の検出）
R. A. Wong, Y. Yokota, M. Wakisaka, J. Inukai, and Y. Kim, J. Am. Chem. Soc., **140**, 13672-13679 (2018).

6. Realization of selective triplet exciton formation in a single molecule [4, 2]
（単分子における三重項励起子の選択的形成の実現）
K. Kimura, K. Miwa, H. Imada, M. Imai-Imada, S. Kawahara, J. Takeya, M. Kawai, M. Galperin, and Y. Kim, Nature, **570**, 210-213 (2019)

7. Development of a theoretical method for describing single-molecule luminescence by STM [4, 2]
（STM を用いた単分子発光分光の理論解析手法の開発）
K. Miwa, H. Imada, M. Imai-Imada, K. Kimura, M. Galperin, and Y. Kim, Nano Lett., **19**, 2803-2811 (2019)

8. Development of single-molecule resonance Raman spectroscopy [4,2]
（単分子共鳴ラマン分光法の開発）
R. B. Jaculbia, H. Imada, K. Miwa, T. Iwasa, M. Takenaka, B. Yang, E. Kazuma, N. Hayazawa, T. Taketsugu, and Y. Kim, Nat. Nanotechnol., **15**, 105-110 (2020)

9. Development of a colorimetric method for detecting pollen allergen using non-crosslinking aggregation of DNA-modified nanoparticles [4]
（DNA 修飾ナノ粒子の非架橋凝集を用いる花粉症アレルゲンの比色検出法の開発）
C. C. Chang, G. Wang, T. Takarada, and M. Maeda, ACS Sens., **4**, 363 (2019)

10. A Nanobiosensor for the Simple Detection of Small Molecules using Non-crosslinking Aggregation of Gold Nanoparticles with G-quadruplexes [4]
（四重鎖 DNA 担持金ナノ粒子の非架橋型凝集に基づく低分子検出ナノバイオセンサーの開発）
S. Chuaychob, C. Thammakhet-Buranachai, P. Kanatharana, P. Thavarungkul, C. Buranachai, M. Fujita, M. Maeda, Anal. Methods., **12**, 230-238 (2020)

11. Iron Dynamics (Reduction, Transport and Sensing) on Biological Membrane-Protein Interface [4]
（細胞膜とタンパク質の界面における生体内鉄動態解析：鉄還元酵素）
M. Ganasen, H. Togashi, H. Takeda, H. Asakura, T. Tosha, K. Yamashita, K. Hirata, Y. Nariai, T. Urano, X. Yuan, I. Hamza, G. A. Mauk, Y. Shiro, H. Sugimoto, H. Sawai: Commun. Biol. **1**: 120 (2018)

12. Iron Dynamics (Reduction, Transport and Sensing) on Biological Membrane-Protein Interface [4]
（細胞膜とタンパク質の界面における生体内鉄動態解析：ヘム膜輸送の分子動力学）
K. Tamura, H. Sugimoto, Y. Shiro, Y. Sugita J. Phys. Chem. B **123**, 7270-7281 (2019)

13. Development of reconfigurable spin filter based on chiral molecular motor driven by light and heat [4]
（キラル分子モーターを用いた光/熱刺激によるスピン偏極スイッチング）
M. Suda, Y. Thathong, V. Promarak, H. Kojima, M. Nakamura, T. Shiraogawa, M. Ehara and H. M. Yamamoto, Nature Commun., **10**, 2455 (2019).

14. Enhanced single photon emission from carbon nanotube dopant states coupled to silicon microcavities [5]
（シリコン微小共振器によるカーボンナノチューブ単一光子発生レートの増強）

A. Ishii, X. He, N. F. Hartmann, H. Machiya, H. Htoon, S. K. Doorn, Y. K. Kato, Nano Lett. **18**, 3873 (2018).

15. Organic molecular tuning of many-body interaction energies in air-suspended carbon nanotubes [5]
（カーボンナノチューブにおける多体相互作用の有機分子吸着による制御）
S. Tanaka, K. Otsuka, K. Kimura, A. Ishii, H. Imada, Y. Kim, Y. K. Kato, J. Phys. Chem. C **123**, 5776 (2019).

16. High efficiency dark-to-bright exciton conversion in carbon nanotubes [5]
（カーボンナノチューブにおける暗い励起子から明るい励起子への高効率変換）
A. Ishii, H. Machiya, Y. K. Kato, Phys. Rev. X **9**, 041048 (2019).

17. Investigation of superconducting phase diagram of an organic Mott insulator using simultaneous control of electric field and strain [5, 1]
（有機モット絶縁体における電界/歪み同時制御による超伝導相の探索）
Y. Kawasugi, K. Seki, S. Tajima, J. Pu, T. Takenobu, S. Yunoki, H.M. Yamamoto, and R. Kato, Science Advances, **5**, eaav7282 (2019).

（４）開発した測定技術・装置 / Developed measuring techniques and equipment (Research Category in [ ])

物質階層原理

1. Apparatus of collinear laser spectroscopy for GeV RI beams [1]
（GeV RI beam 用コリニア分光装置）
2. Apparatus for β-ray-detected NMR spectroscopy [1, 3]
（β 線検出型核磁気共鳴装置）
3. β-Ray-detected NMR method utilizing spin-aligned RI beams [1]
（核スピン整列 RI ビームを用いた β 線検出型 NMR 測定法）
4. Cryogenic ion storage ring (RICE) [1, 2]
（極低温イオン蓄積リング）
5. Neutral atomic beam [1, 2]
（中性原子ビーム生成装置）
6. Application of TES（Transition Edge Sensor）for the exotic atom experiment [1, 2]
（超伝導転移点カロリメータ TES を用いたエキゾチック原子 X 線検出技術）
7. Cryogenic ion trap [1, 2]
（極低温イオントラップ）

8. DAC（Diamond Anvil Cell）technique for resistivity measurements under high pressure [1]
（DAC を用いた超高圧下抵抗測定技術）

9. Sub-terahertz ESR measurement system [1]
（サブテラヘルツ波 ESR 測定装置）

10. ROS (Reactive Oxygen Species) evaluation apparatus for biological materials using ESR [1]
（ESR を利用した ROS 評価装置）

11. Magnetic torque measurement system using MEMS (Micro Electro Mechanical Systems) [1]
（MEMS を用いた磁気トルク測定装置）

12. Colloidal probe atomic force microscopy for measurement of interfacial forces between brush-like DNA layers [1]
（コロイドプローブ原子間力顕微鏡を用いた DNA ブラシ層間相互作用測定技術）

13. Optical tweezers for measurement of DNA-DNA interactions at the single-molecule level [1]
（光ピンセットを用いた DNA 単分子間相互作用測定技術）

14. Microfluidic system for movement observation of micro-organs with multiple tactic stimuli [1]
（多重刺激下の微生物の動きを観察するマイクロ流路システム）

15. Optical feedback system constructed for movement analysis of gene-modified micro swimmers (Euglena gracilis) [1]
（遺伝子操作したマイクロスイマーへの光学フィードバック装置）

16. Image-analysis software for long-term evolution in phototaxis, chemotaxis, or gravitaxis of Euglena cells confined in a microfluidic chip [1]
（マイクロ流路中の微生物の化学走性と重力走性の長時間イメージ解析ソフトウェア）

17. Techniques using the Caged Compounds for Characterization of Short-lived Reaction Intermediates [1]
（ケージド化合物を用いた酵素反応の短寿命反応中間体の電子状態・構造解析法）

18. Electrospray-cold ion trap laser spectrometer [1, 4]
（エレクトロスプレー－冷却イオントラップレーザー分光装置）

19. Highly nuclear-spin-aligned RI beams produced by a two-step nuclear reaction combined with the momentum-dispersion matching technique [2]
（分散整合二回散乱法による核スピン整列 RI ビーム生成技術）

20. Deep-UV femtosecond stimulated Raman spectroscopy (DUV-FSRS) [2]
（深紫外フェムト秒誘導ラマン分光法）

21. Dynamic quenching two-dimensional fluorescence lifetime correlation spectroscopy (DQ 2D-FLCS) [2]
（動的消光二次元蛍光寿命相関分光）

22. Controlling of plasmon-induced single-molecule reaction [2]
（プラズモンによる単分子反応制御技術）

23. High-throughput, trigger-less data acquisition system [2,1]
（高効率トリガレスデータ収集システム）

24. High-rate, high-time resolution beam counter with a Cherenkov radiator [2,1]
（チェレンコフ輻射体を用いた高速高時間分解能ビーム計数器）

25. High-rate scintillation fiber tracker [2,1]
（シンチレーションファイバーを用いた高速粒子飛跡検出器）

ヘテロ界面

1. Optical radioisotope atom observation in condensed helium as ion-catcher system (OROCHI) [3, 2, 1]
（凝縮体ヘリウムをトラップ媒質とした RI 原子の新奇レーザー分光装置）

2. Electron cyclotron resonance ion source [3]
（電子サイクロトロン共鳴型（ECR）イオン源）

3. Cryogenic nozzle for large helium droplet production [3]
（巨大ヘリウム液滴生成用極低温ノズル）

4. UV-excited time-resolved heterodyne-detected vibrational sum-frequency generation (UV TR-HD-VSFG) [4]
（紫外励起時間分解ヘテロダイン振動和周波発生分光法）

5. Single-molecule absorption spectroscopy [4]
（単分子吸収分光法）

6. Single-molecule resonance STM tip-enhanced Raman spectroscopy [4]
（単分子共鳴探針増強ラマン分光法）

7. Controlled formation of triplet exciton in a single molecule [4]
（単分子における励起子形成の制御手法）

8. Semi-in-situ method for chemical characterization of the electrical double layer at the electrode surface [4]
（電極表面における電気二重層の semi-in-situ 化学同定手法）

9. Simultaneous control of the bandfilling and bandwidth using electric field doping and substrate bending at a device interface [5, 1]
（デバイス界面において、電界ドーピングと基板曲げひずみを用いたバンド占有率とバンド幅の同時制御する技術）

10. Time-resolved and photon correlation measurement with a fully-automated telecom-band photoluminescence microscopy system [5]
（全自動通信波長帯フォトルミネッセンス顕微分光システムによる時間分解および光子相関測定）

（５）セミナー・シンポジウム / Seminars and Symposiums

2017 年度

・「物質階層の原理を探求する総合的実験研究」第 1 回春期研究会
2017 年 5 月 12 日−13 日、御殿場高原ホテル

・「物質階層の原理を探求する総合的実験研究」研究報告会
2018 年 2 月 13 日−14 日、理化学研究所 鈴木梅太郎ホール

・第 1 回 ExpRes Dojo “Laser”
2017 年 6 月 16 日、理化学研究所 鈴木梅太郎ホール

・第 2 回 ExpRes Dojo “Data Acquisition”
2017 年 10 月 6 日、理化学研究所 大河内ホール

2018 年度

・「物質階層原理研究」&「ヘテロ界面研究」合同春合宿
2018 年 5 月 11 日−12 日、かんぽの宿 熱海本館

・「物質階層原理研究」&「ヘテロ界面研究」研究報告会
2019 年 2 月 5 日−6 日、理化学研究所 鈴木梅太郎ホール

・第 3 回 ExpRes Dojo “サルでもわかる量子コンピューター”、見学会
2018 年 6 月 8 日、理化学研究所 鈴木梅太郎ホール

・第 4 回 ExpRes Dojo “Precision Detection / Detector”
2017 年 10 月 5 日、理化学研究所 RIBF conference room

2019 年度

・「物質階層原理研究」&「ヘテロ界面研究」合同春合宿
2019 年 5 月 10 日−11 日、御殿場高原ホテル

・「物質階層原理研究」&「ヘテロ界面研究」研究報告会
2020 年 2 月 4 日−5 日、理化学研究所 鈴木梅太郎ホール

・第 5 回 ExpRes Dojo “測定を支える基本要素 Sample & Probe”
2020 年 1 月 14 日、理化学研究所 RIBF conference room

詳細は、次ページ以降

「物質階層の原理を探求する統合的実験研究」

第 1 回春期研究会

2017 年 5 月 12 日（金）－13 日（土）

於　御殿場高原ホテル（静岡県御殿場市神山 719）

1 日目：2017 年 5 月 12 日（金）

13:00－13:20　はじめに（加藤 礼三）

【座長：東 俊行】

13:20－13:50　O-01　宇宙における化学進化の解明のための地上実験に向けて
中野 祐司（東原子分子物理研究室）

13:50－14:20　O-02　原子スペクトルの精密分光による超変形原子核探索
高峰 愛子（上野核分光研究室）

14:20－14:50　O-03　Study of the lightest kaonic nuclei at J-PARC
山我 拓巳（大阪大学）

14:50－15:10　休憩

【座長：岩崎 雅彦】

15:10－15:50　O-04　原子核物理学の観点からの物質階層
肥山 詠美子（肥山ストレンジネス核物理研究室）

15:50－16:30　O-05　フェルミ多粒子系ダイナミクスのシミュレーション
矢花 一浩（筑波大学計算科学研究センター）

【座長：加藤 礼三】

16:30－17:15　パネルディスカッション
「物質科学における異分野連携」

17:15－18:00　自由討論

18:00－20:00　意見交換会

20:00－22:00　ポスターセッション

2 日目：2017 年 5 月 13 日（土）

【座長：金 有洙】

9:30－10:00　O-06　電子スピン共鳴を用いた分子性物質の研究
大島 勇吾（加藤分子物性研究室）

10:00－10:30　O-07　プラズモン誘起化学反応の実空間・実時間観測
數間 惠弥子（Kim 表面界面科学研究室）

10:30－10:50　休憩

【座長：田原 太平】

10:50－11:20　O-08　界面選択的非線形分光による界面科学の深化
二本柳 聡史（田原分子分光研究室）

11:20－11:50　O-09　病原菌の細胞膜で機能するヘム輸送タンパク質の構造と機能
杉本 宏（兵庫県立大/ビームライン基盤研究部）

11:50－13:10　昼食

【座長：城 宜嗣】

13:10－13:40　O-10　Characterizing nitric oxide diffusion in a nitrite reductase: Nitric oxide reductase complex
Pohung Wang（杉田理論分子科学研究室）

13:40－14:20　O-11　量子散逸系のダイナミクス理論とその光合成初期過程への展開
石崎 章仁（分子科学研究所）

14:20－14:40　休憩

【座長：前田 瑞夫】

14:40－15:10　O-12　DNA 修飾金ナノ粒子集合体の構造変換
宝田 徹（前田バイオ工学研究室）

15:10－15:50　O-13　合成生物学:生命システムを数理モデルに基づいて設計・実装して理解する
木賀 大介（早稲田大学理工学術院 電気・情報生命工学科）

15:50　終わりに（上野 秀樹）

ポスター発表（5 月 12 日夜）

P-01　ナノ細孔を有する分子性導体の開発
井口 弘章（東北大学錯体化学研究室）

P-02　一分子蛍光計測に立脚した生体高分子の構造ダイナミクスの研究
石井 邦彦（田原分子分光研究室）

P-03　ボトムアップアプローチによる神経伝達過程の分子選択性の解明
石内 俊一（東京工業大学科　学技術創成研究院　化学生命科学研究所）

P-04　室温エネルギーミュオン源の開発とその応用
石田 勝彦（岩崎先端中間子研究室）

P-05　磁気トルクで見た三角格子有機磁性体の量子スピン液体状態
磯野 貴之（加藤分子物性研究室）

P-06　Real-space investigation of intermolecular energy transfer dynamics
今田 裕（Kim 表面界面科学研究室）

P-07　超伝導検出器を用いた原子分子ビーム計測に向けて
岡田 信二（東原子分子物理研究室）

P-08　イオン液体トランジスタによる分子性導体の超伝導相の探索
川椙 義高（加藤分子物性研究室）

P-09　Precision microwave spectroscopy of muonium atom
神田 聡太郎（岩崎先端中間子研究室）

P-10　Valence bond solid 物質 $EtMe_3P[Pd(dmit)_2]_2$ の電子スピン共鳴
金 星賢（加藤分子物性研究室）

P-11　極低温分子イオンのダイミクス解明に向けて
久間 晋（東原子分子物理研究室）

P-12　超高速時間領域ラマン分光法で観る光応答性タンパク質の反応初期過程
倉持 光（田原分子分光研究室）

P-13　超高圧下による単一成分分子性結晶[Pt(dddt)$_2$]の金属化
崔 亨波（加藤分子物性研究室）

P-14　キセノン原子 EDM 測定へ向けた能動帰還型核スピンメーザーの開発
佐藤 智哉（上野核分光研究室）

P-15　Optical isomer separation by FEL ＆ ultra low energy electron scattering from N_2O
佐山 篤（田原分子分光研究室）

P-16　光誘起界面双極子を利用した光駆動型有機超伝導トランジスタの開発
須田 理行（分子科学研究所）

P-17　Vibrational analysis of aromatic polyamide reverse osmosis membranes
Surblys Donatas（杉田理論分子科学研究室）

P-18　時間分解分光法を用いた一酸化窒素還元酵素の触媒反応機構の解明
武田 英恵（兵庫県立大理学部）

P-19　ハイブリッド汎関数法による分子性導体の磁性と電子状態
圓谷 貴夫（物質・材料研究機構）

P-20　SACLA を利用した時間分解 X 線結晶構造解析による酵素反応の観測
當舍 武彦（兵庫県立大/ビームライン基盤研究部）

P-21　核スピン偏極を用いた原子核構造研究
西畑 洸希（上野核分光研究室）

P-22　環境制御下での先端増強ラマン分光法の開発
早澤 紀彦（Kim 表面界面科学研究室）

P-23　ABC ヘム排出ポンプの構造と機能
久野 玉雄（ビームライン基盤研究部）

P-24　レーザー・マイクロ波二重共鳴法による超流動ヘリウム環境中 Au 原子の超微細構造間隔
藤田 朋美（上野核分光研究室）

P-25　DNA ナノ粒子の分散・凝集と枯渇効果
藤田 雅弘（前田バイオ工学研究室）

P-26　バンドギャップ内に存在する連続磁気励起
藤山 茂樹（加藤分子物性研究室）

P-27　Organic superconductor λ-$(BETS)_2GaCl_4$ study by Muon spin rotation
Puspita Sari Dita（岩崎先端中間子研究室）

P-28　低次元金属錯体におけるバンドフィリング制御と熱電特性の評価
村杉 英昭（東北大学錯体化学研究室）

P-29　QM/MM 法に基づく反応経路探索法の開発と酵素反応への応用
八木 清（杉田理論分子科学研究室）

P-30　一酸化窒素還元酵素の基質輸送経路に存在するアミノ酸残基の役割
山際 来佳（兵庫県立大理学部）

P-31　NOR が関わる複合体の構造安定性と機能の理論解析
山田 健太（杉田理論分子科学研究室）

P-32　Self-organization of DNA-coated gold nanoparticle assemblies through non-crosslinking aggregation
余 力（前田バイオ工学研究室）

P-33　電気化学界面の探針増強ラマン分光
横田 泰之（Kim 表面界面科学研究室）

P-34　Observation of the anomalous antiferromagnetic resonance in λ-$(BETS)_2FeCl_4$
李 泰勳（加藤分子物性研究室）

P-35　DNA 修飾金ナノ粒子集合体の配向制御
王 国慶（前田バイオ工学研究室）

「物質階層の原理を探求する統合的実験研究」

研究報告会

2018 年 2 月 13 日（火）－14 日（水）

於　理化学研究所 鈴木梅太郎ホール

1 日目：2018 年 2 月 13 日（火）

13:20－13:30　開会挨拶（小安 重夫 理事）

13:30－13:40　概要説明（加藤 礼三）

【座長：前田 瑞夫】

13:40－14:25　I-1　SACLA 自由電子レーザーによる膜タンパク質の構造の分子動画撮影
岩田 想（SACLA 利用技術開拓グループ／京都大学）

14:25－14:50　O-1　生体内鉄動態：生体膜を通した鉄の取り込み
城 宜嗣（兵庫県立大学）

14:50－15:05　休憩

【座長：城 宜嗣】

15:05－15:50　I-2　クライオ電子顕微鏡単粒子解析による電位依存性チャネルの構造解析
重松 秀樹（ライフサイエンス技術基盤研究センター）

15:50－16:15　O-2　DNA を用いるナノ粒子集合体の配向制御
前田 瑞夫（前田バイオ工学研究室）

16:15－16:30　休憩

【座長：田原 太平】

16:30－17:15　I-3　量子化学研究の最新の展開：振動状態理論・反応経路網・ダイナミクス
武次 徹也（北海道大学）

17:15－17:40　O-3　単一分子におけるエネルギー移動・変換
金 有洙（Kim 表面界面科学研究室）

18:00－20:00　意見交換会（広沢クラブ）

2 日目：2018 年 2 月 14 日（水）

【座長：金 有洙】

9:15－10:00　I-4　星間雲の階層構造と化学
山本 智（東京大学）

10:00－10:25　O-4　光受容タンパク質のフェムト秒構造変化の観測とその生物的機能発現における意味
田原 太平（田原分子分光研究室）

10:25－10:40　休憩

【座長：東 俊行】

10:40－11:25　I-5　量子クラスターで読み解く物質の階層構造
中村 隆司（東京工業大学）

11:25－11:50　O-5　K 中間子束縛核探査実験
岩崎 雅彦（岩崎先端中間子研究室）

11:50－12:15　O-6　GeV RI ビームを用いた新なレーザー核分光装置の開発
上野 秀樹（上野核分光研究室）

12:15－13:30　昼食

【座長：岩崎 雅彦】

13:30－14:15　I-6　冷却原子気体を用いた極低温量子物質の実験的シミュレーション
堀越 宗一（東京大学）

14:15－14:40　O-7　真空中に孤立した分子の excitation と dynamics の解明に向けて
東 俊行（東原子分子物理研究室）

14:40－14:55　休憩

【座長：上野 秀樹】

14:55－15:40　I-7　固体における創発性粒子 － スキルミオン
永長 直人（創発物性科学研究センター）

15:40－16:05　O-8　分子性量子スピン液体におけるスピン・電荷・軌道・格子自由度
加藤 礼三（加藤分子物性研究室）

16:05－16:10　終わりに


12:28

ExpRes Dojo 道場 “LASER”

Pioneering Project “Fundamental Principles Underlying the Hierarchy of Matter: A Comprehensive Experimental Study”

独創的研究提案課題「物質階層の原理を探求する統合的実験研究」

Date: June 16 (Fri.), 2017

13:00-18:00

Venue: Suzuki Umetaro Hall

13:00 – 13:10	はじめに（東　俊行）
[座長] 岩崎	
13:10 - 13:40	XFEL と赤外レーザーを用いた生体分子のダイナミクス研究 久保　稔　（放射光科学総合研究センター　イメージングチーム）
13:40 – 14:10	プラズモニックナノ光源による顕微分光法 早澤　紀彦　(Kim 表面界面科学研究室)
14:10 - 14:40	超高速分光を可能にする様々なレーザー光源と光技術 竹内　佐年（田原分子分光研究室）
14:40 - 15:00	*Coffee Break*
[座長]　城	
15:00 - 15:30	様々なレーザー光源によるイオントラップやイオンリングに蓄積された分子イオンの分光とダイナミクス研究 Sebastian Menk (首都大学東京，東原子分子物理研究室)
15:30 - 16:00	超流動ヘリウム中に埋め込まれた原子のレーザー分光とその核構造研究への応用 今村慧（岡山大，上野核分光研究室）
16:00 - 16:30	パルスライマンアルファレーザー 大石 裕（KEK，岩崎先端中間子研究室）
16:30 - 16:50	*Coffee Break*
[座長]　金	
16:50 - 17:20	オンデマンドレーザーの開発と今後の展開 和田 智（光量子工学研究領域，光量子制御技術開発チーム）
17:20－17:50	パネルディスカッション
17:50 - 18:00	終わりに（加藤 礼三）
18:00－20:00	意見交換会　　第一食堂にて

第２回　ExpRes Dojo 道場
“Data Acquisition”

Pioneering Project “Fundamental Principles Underlying the Hierarchy of Matter: A Comprehensive Experimental Study”

独創的研究提案課題「物質階層の原理を探求する統合的実験研究」

Date:　Friday, October 6, 2017　2017 年 10 月 6 日（金）
Venue: Okouchi Hall　大河内ホール

13:30 – 13:40　はじめに Opening Remarks（上野 秀樹 Dr. Ueno）

［座長 Chairperson：東 Dr. Azuma］

13:40 – 14:10　生体分子ダイナミクス計測のための光子データ解析
Photon data analysis for measuring dynamics of biomolecules
石井 邦彦 Dr. Ishii（田原分子分光研究室 *Molecular Spectroscopy Lab.*）

14:10 – 14:40　原子・分子・光物理実験におけるデータ取得と解析
Data acquisition and analysis in atomic, molecular and optical physics experiments
久間 晋 Dr. Kuma（東原子分子物理研究室 *Atomic, Molecular and Optical Physics Lab.*）

14:40 – 15:00　休憩 Coffee Break

［座長 Chairperson：加藤 Dr. Kato］

15:00 – 15:30　J-PARC 物質・生命科学実験施設のデータ収集システム
Data acquisition system at the Materials and Life science experimental Facility of J-PARC
中谷 健 Dr. Nakatani（日本原子力研究開発機構 J-PARC センター *JAEA, J-PARC Center*）

15:30 – 16:00　Prototyping for a trigger-less DAQ at J-PARC
Dr. Yue Ma（岩崎先端中間子研究室 *Advanced Meson Science Lab.*）

16:00 – 16:20　休憩 Coffee Break

［座長 Chairperson：金 Dr. Kim］

16:20 – 16:50　理研 RIBF でのデータ収集システムと関連技術の紹介
Data acquisition system in RIKEN RIBF and related technologies
馬場 秀忠 Dr. Baba（仁科加速器研究センター 情報処理技術チーム *Nishina Center*）

16:50 – 17:20　放射光・XFEL のデータ取得技術
Wide-band Data Acquisition at Synchrotron Radiation and X-ray Free-Electron Laser experiments
初井 宇記 Dr. Hatsui（SPring-8 データ処理系開発チーム *SPring-8 Center*）

17:20 – 17:50　パネルディスカッション Panel Discussion

17:50 – 18:00　終わりに Closing Remarks（岩崎 雅彦 Dr. Iwasaki）

18:00 – 20:00　意見交換会 After-Symposium Exchange Meeting ［第１食堂 Main Cafeteria］

「物質階層原理研究」&「ヘテロ界面研究」合同春合宿

日時：2018 / 5 / 11（金）　13：00 – 22：00
　　5 / 12（土）　9：30 – 15：20
場所：かんぽの宿 熱海本館（静岡県熱海市水口町 2-12-3）

プログラム

Time table（May 11）

13:00 - 13:05　はじめに
加藤　礼三（理化学研究所　加藤礼三分子物性研究室）

13:05 – 13:15　ヘテロ界面概要説明
金　有洙（理化学研究所　Kim 表面界面科学研究室）

Chair – 金　有洙

13:15 - 13:55　O-01　糖鎖の不均一性による生体内パターン認識
田中　克則（理化学研究所　田中生体機能合成化学研究室）

13:55 - 14:25　O-02　電気化学界面の微視的理解に向けた In situ 及び Ex situ 手法の開発
横田　泰之（理化学研究所　Kim 表面界面科学研究室）

14:25 - 14:55　O-03　二次元蛍光寿命相関分光法を用いた生体高分子の構造形成機構の研究
石井　邦彦（理化学研究所　田原分子分光研究室）

14:55 - 15:15　Coffee break

Chair – 岩崎　雅彦

15:15 - 15:55　O-04　レーザー冷却原子・イオン混合系で探究する極低温物理
向山　敬（大阪大学　基礎工学研究科）

15:55 - 16:25　O-05　超流動ヘリウム液滴中で探る低温分子イオンの物理
久間　晋（理化学研究所 東原子分子物理研究室）

16:25 - 16:55　O-06　超流動ヘリウム中原子の超高速分光測定によるダイナミクス研究へ向けて
松尾　由賀利（法政大学理工学部）

16:55 - 17:15　Coffee break

Chair – 加藤　雄一郎

17:15 - 17:55　Panel discussion
パネラー　山本　浩史（分子科学研究所）
高峰　愛子（理化学研究所　仁科加速器科学研究センター 核分光研究室）
横田　泰之（理化学研究所　Kim 表面界面科学研究室）
梅野　太輔（千葉大学大学院工学研究院）
神田　聡太郎（理化学研究所　仁科加速器科学研究センター 中間子研究室）
金　栄鎮（理化学研究所　前田バイオ工学研究室）

17:55 - 18:00　Break

18:00 - 20:00　意見交換会（at 大広間）
20:00 - 22:00　Poster session（at サンレモ）

Time table（May 12）

Chair - 加藤　礼三

9:30 - 10:10　O-07　氷における水分子の配向秩序と表面での構造乱れ
松本　吉泰（豊田理化学研究所）

10:10 - 10:40　O-08　磁気熱量測定による有機三角格子磁性体における量子スピン液体の研究
磯野　貴之（理化学研究所　加藤礼三分子物性研究室）

10:40 - 11:10　O-09　Room-temperature single photon emission from carbon nanotubes
石井　晃博（理化学研究所　加藤ナノ量子フォトニクス研究室）

11:10 - 11:30　Coffee break

Chair – 上野　秀樹

11:30 - 12:10　O-10　重いクォークを探針としてバリオン内部のクォークの動きを探る
野海　博之（大阪大学　核物理研究センター）

12:10 - 12:40　O-11　K 中間子原子核探索実験の現状、及び、今後の展開
佐久間　史典（理化学研究所　仁科加速器科学研究センター　中間子研究室）

12:40 - 13:30　Lunch

Chair – 田原　太平

13:30 - 14:10　O-12　センサと制御ネットワーク機能の「生まれ方」
梅野　太輔（千葉大学大学院工学研究院）

14:10 - 14:40　O-13　Laminar flow dendritic amplification-assisted microRNA detection on a power-free microfluidic chip
金　栄鎮（理化学研究所　前田バイオ工学研究室）

14:40 - 15:10　O-14　ヒトの鉄吸収機構を原子・分子 ⇔ 細胞・組織の階層で相互に理解する
澤井　仁美（兵庫県立大学　大学院生命理学研究科）

15:10 - 15:20　おわりに

Poster session (5/11 night)

P-01 Studying Negative Ions in Cryogenic Electrostatic Ion Storage Rings
Kiattichart　Chartkunchand（Atomic, Molecular, and Optical Physics Laboratory）

P-02 枯渇効果で見る DNA ナノ粒子の分散安定性
藤田　雅弘（理化学研究所　前田バイオ工学研究室）

P-03 先端増強ラマン分光法による極限的空間分解能への挑戦
早澤　紀彦（理化学研究所　Kim 表面界面科学研究室）

P-04 STM を用いた分子系エネルギーダイナミクスの研究
今田　裕（理化学研究所　Kim 表面界面科学研究室）

P-05 ニュートリノ質量分光へ向けた 3 光子放出過程の増幅実験
今村　慧（岡山大学　異分野基礎科学研究所　量子宇宙研究コア）

P-06 エレクトロスプレー・冷却イオントラップ法による
K+イオンチャンネル部分ペプチド・アルカリ金属イオン錯体の赤外分光
石内　俊一（東京工業大学化学生命科学研究所）

P-07 ミュオン水素原子の精密レーザー分光による陽子半径の測定
神田　聡太郎（理化学研究所　仁科加速器科学研究センター　中間子研究室）

P-08 核破砕反応を用いた高スピンアイソマーの生成
川田　敬太（理化学研究所　仁科加速器科学研究センター　核分光研究室）

P-09 単一分子プラズモン誘起化学反応の実空間・実時間観測
數間　惠弥子（理化学研究所　Kim 表面界面科学研究室）

P-10 アト秒精度で制御されたパルス対によるフーリエ変換 2 次元電子分光
倉持　光（理化学研究所　田原分子分光研究室）

P-11 波長領域における空気モードナノビーム共振器と単一カーボンナノチューブの光結合の制御
町屋　秀憲（理化学研究所　加藤ナノ量子フォトニクス研究室）

P-12 λ-(STF)2GaCl4 の圧力下超伝導相と隣接する常磁性相の磁気的性質
南舘　孝亮（理化学研究所　加藤分子物性研究室）

P-13 スピン偏極 23Ne を用いた ZnO 単結晶電場勾配測定
西畑　洸希（理化学研究所　仁科加速器科学研究センター　核分光研究室）

P-14 ミリ波を用いた電子スピン共鳴／サイクロトロン共鳴装置の開発
大島　勇吾（理化学研究所　加藤分子物性研究室）

P-15 同位体プログラミングによる単層カーボンナノチューブの成長過程追跡
大塚　慶吾（理化学研究所　量子オプトエレクトロニクス研究チーム）

P-16 ユーグレナの青色光忌避応答のシグナルパス
尾笹　一成（理化学研究所　前田バイオ工学研究室）

P-17 能動帰還型核スピンメーザーを用いたスピン歳差周波数測定における誤差とその低減
佐藤 智哉（理化学研究所　仁科加速器科学研究センター　核分光研究室）

P-18 入射核破砕反応で得られる不安定核ビームに対するコリニアレーザー分光装置の開発
田島　美典（理化学研究所　仁科加速器科学研究センター　核分光研究室）

P-19 RF トラップの原理を応用した超低速不安定核ビーム生成装置の開発
高峰 愛子（理化学研究所 仁科加速器科学研究センター　核分光研究室）

P-20 Ne 二量体の二光子吸収二電子励起による原子間クーロン緩和過程の時間分解測定
高梨　司（理化学研究所　田原分子分光研究室）

P-21 DNA 修飾ナノ粒子集合体の会合操作
宝田　徹（理化学研究所　前田バイオ工学研究室）

P-22 時間分解可視・赤外吸収分光を用いた一酸化窒素還元酵素が触媒する NO 還元反応の直接観測
武田　英恵（兵庫県立大学大学院　生命理学研究科　生命科学専攻）

P-23 Molecular screening effects on trion binding energies and electronic band gaps in air-suspended carbon nanotubes
田中　駿介（理化学研究所　加藤ナノ量子フォトニクス研究室）

P-24 トリフェニルアミン骨格を持つ混合原子価分子の電荷/スピン移動
上辺　将士（理化学研究所　加藤分子物性研究室）

P-25 超流動ヘリウム中 In 原子の偏極生成に向けたパルス Ti:Sa レーザーの開発
矢田　智昭（法政大学大学院 理工学研究科）

P-26 QM/MM 法に基づく生体分子の非調和振動解析
八木　清（理化学研究所　杉田理論分子科学研究室）

2018 年度

「物質階層原理研究」＆「ヘテロ界面研究」

研究報告会

2019 年 2 月 5 日（火）－6 日（水）

於　理化学研究所 鈴木梅太郎ホール

1 日目：2019 年 2 月 5 日（火）

13:30－13:40　概要説明（加藤 礼三）

【座長：城 宜嗣】

13:40－14:25　I-1　高速一分子蛍光分光法によるタンパク質の構造形成ダイナミクス
高橋 聡（多元物質科学研究所／東北大学）

14:25－14:55　O-1　二次元蛍光寿命相関分光による RNA リボスイッチのマイクロ秒領域の折り畳み機構
田原 太平（田原分子分光研究室）

14:55－15:20　O-2　冷却イオン分光による天然変性タンパク質
-低分子リガンド複合体へのボトムアップアプローチ
藤井 正明（科学技術創成研究院／東京工業大学）

15:20－15:35　休憩

【座長：田原 太平】

15:35－16:20　I-2　光受容型膜タンパク質・微生物型ロドプシンの物理化学研究
井上 圭一（物性研究所／東京大学）

16:20－16:50　O-3　生体内鉄動態：生体膜を通した鉄の取り込み
城 宜嗣（生命理学研究科／兵庫県立大学）

16:50－17:20　O-4　単層カーボンナノチューブの明るい励起子と暗い励起子
加藤 雄一郎（加藤ナノ量子フォトニクス研究室）

17:45－19:45　意見交換会（広沢クラブ）

2 日目：2019 年 2 月 6 日（水）

【座長：上野 秀樹】

9:15－10:00　I-3　光格子重元素干渉計による基本対称性の破れの研究
酒見 泰寛（原子核科学研究センター／東京大学）

10:00－10:30　O-5　孤立分子イオンの放射冷却過程
東 俊行（東原子分子物理研究室）

10:30－10:45　休憩

【座長：東 俊行】

10:45－11:15　O-6　分野間技術連携による原子・核物理境界領域研究
上野 秀樹（上野核分光研究室）

11:15－11:45　O-7　原子核の中の階層構造とその新展開
岩崎 雅彦（岩崎先端中間子研究室）

11:45－12:10　O-8　重いクォークを含むバリオン励起状態の研究
野海 博之（核物理研究センター／大阪大学）

12:10－13:35　昼食

【座長：加藤 雄一郎】

13:35－14:20　I-4　ナノ構造の光学応答と光圧操作
石原 一（物質創成専攻未来物質領域／大阪大学）

14:20－14:50　O-9　局所界面におけるエネルギー移動・変換・散逸過程の理解：
表面プラズモンによる単一分子化学反応の制御
金 有洙（Kim 表面界面科学研究室）

14:50－15:15　O-10　分子ヘテロ界面を用いた電子デバイス研究
山本 浩史（協奏分子システム研究センター／分子科学研究所）

15:15－15:30　休憩

【座長：金 有洙】

15:30－16:00　O-11　単一成分分子性導体の開発
加藤 礼三（加藤分子物性研究室）

16:00－16:30　O-12　DNA 間相互作用に基づくナノ粒子の組織化
前田 瑞夫（前田バイオ工学研究室）

16:30－16:40　閉会挨拶（小安 重夫 理事）

16:40－16:45　終わりに（金 有洙）

第３回ExpRes道場

A Joint Workshop of Pioneering Projects,
"Fundamental Principles Underlying the Hierarchy of Matter: A Comprehensive Experimental Study"
「物質階層の原理を探求する統合的実験研究」 &
"Heterogeneity at Materials Interfaces"「ヘテロ界面研究」

2018年6月8日（金）
鈴木梅太郎ホール

13:00 - 13:10 はじめに（金 有洙）
13:10 - 14:00 特別講義「サルでもわかる量子コンピューター」
大野圭司（石橋極微デバイス工学研究室）
14:00 - 14:30 見学対象研究室からの概要説明（3分ずつ、研究テーマと場所について）
14:40 - 16:10 南地区の研究室（加藤研、前田研、田原研、Kim研）の見学
14:40 - 15:20 1st round
15:30 - 16:10 2nd round
16:30 - 18:00 研究本館（加藤（雄）研、岩崎研、）、レーザー棟（東研、上野研）、仁科（上野研）の見学
16:30 - 17:10 1st round (上野研はRIBFのみ)
17:20 - 18:00 2nd round (上野研はレーザー棟のみ)
18:00 - 金酒（自由討論）

見学場所及び担当者
金研（ナノ棟）；横田　加藤（礼）研（物質棟）；大島　田原研（物質棟）；石井　前田研（交流棟）；藤田
加藤（雄）研（研究本館）；石井　岩崎研（研究本館）；石田　東研（レーザ棟）；久間　上野研（RIBF棟、レーザー棟）；田島

第4回　ExpRes Dojo 道場 “Precision Detection / Detector”

A Joint Workshop of Pioneering Projects,

“Fundamental Principles Underlying the Hierarchy of Matter: A Comprehensive Experimental Study”

「物質階層の原理を探求する統合的実験研究」 &

“Heterogeneity at Materials Interfaces”「ヘテロ界面研究」

Date: October 5 (Fri.), 2018

13:00 – 17:10

Venue: RIBF Conference Room (2F)

13:00 – 13:10	はじめに（岩崎 雅彦）
[座長] 上野	
13:10 – 13:50	「Non-destructive detection of a single antiproton in a Penning trap」 電磁トラップ中の反陽子一粒子の非擾乱計測 長濱 弘季（東大CNS）
13:50 – 14:30	「高エネルギー宇宙観測に用いる検出器」 ″X-ray and gamma-ray detectors for high energy astrophysics” 玉川 徹（理研・高エネルギー宇宙物理研究室）
14:30 – 15:10	「超伝導転移端センサーによるX線精密分光と低速中性分子測定」 Precision spectroscopy of X-ray & cold-neutral molecule via Superconducting Transition Edge Sensor (TES) 岡田 信二（理研・東原子分子物理研究室）
15:10 – 15:40	----- Coffee Break -----
[座長] 加藤(雄)	
15:40 – 16:20	「マイクロカンチレバーを用いた精密物性測定」 Physical properties measurement with micro-cantilever 大島 勇吾（理研・加藤分子物性研究室）
16:20 – 17:00	「Imaging of nanoscale electron dissipation via THz fluctuation」 THz揺らぎによるナノスケール電子消散イメージング Qianchun Weng（東大）
17:00 – 17:10	終わりに（加藤 礼三）
17:30－19:30	意見交換会　　第一食堂にて

「物質階層原理研究」&「ヘテロ界面研究」
合同春合宿
2019 年 5 月 10 日（金）～11 日（土）

於　御殿場高原ホテル Hotel Brush Up（**静岡県御殿場市神山** 719）

1 日目：2019 年 5 月 10 日（金）

13:00～13:05　　はじめに（物質階層原理研究）加藤　礼三
13:05～13:10　　はじめに（ヘテロ界面研究）金　有洙

【座長：上野　秀樹】

13:10～13:45　　O-01 高橋　忠幸（東京大学）
宇宙観測ガンマ線イメージング技術の異分野への応用

13:45～14:10　　O-02 市川　雄一（上野核分光研究室）
原子核励起状態の磁気モーメント測定

14:10～14:35　　O-03 木村　直樹（東原子分子物理研究室）
多価イオン可視光遷移の精密分光法開発

14:35～14:55　　休憩

【座長：加藤　雄一郎】

14:55～15:20　　O-04 崔　亨波（加藤分子物性研究室）
超高圧下による単一成分分子性結晶の物性探索

15:20～15:45　　O-05 田中駿介（加藤ナノ量子フォトニクス研究室）
Organic molecular tuning of many-body interaction energies in air-suspended carbon nanotubes

15:45～16:20　　O-06 高橋　真木子（金沢工業大学）
「企業現場と基礎研究の出会い。」
～出会えるの？出会わないといけない？？出会ってしまったらどうする？？～

16:20～16:45　　集合写真＋休憩

【モデレーター：高橋　真木子】

16:45～17:30　　パネルディスカッション

「企業現場と基礎研究の出会い」

徳田　真（株式会社生命科学インスティテュート）

梅垣　いづみ（豊田中央研究所）

岡田　智成（花王株式会社　スキンケア研究所）

木村　直樹（東原子分子物理研究室・前職コニカミノルタ株式会社）

17:30～18:00　　チェックイン

18:00～20:00　　意見交換会

20:00～22:00　　ポスターセッション

2 日目：2019 年 5 月 11 日（土）

【座長：岩崎　雅彦】

9:30～9:55　　O-07 神田　聡太郎（岩崎中間子研究室）

ミュオン水素原子のレーザー分光による陽子 Zemach 半径の測定

9:55～10:20　　O-08 Ma Yue（岩崎中間子研究室）

A possible ultra-solution for the data taking task in Experimental Physics

10:20～10:40　　休憩

【座長：東　俊行】

10:40～11:15　　O-09 安達　千波矢（九州大学）

有機半導体における電流励起下での励起子過程と発光デバイスへの応用

11:15～11:40　　O-10 今井みやび（Kim 表面界面科学研究室）

STM 発光分光法を用いたフタロシアニン単一分子内での励起子生成・消滅過程の可視化

11:40～13:00　　昼食

【座長：城　宜嗣】

13:00～13:35　　O-11 佐藤　守俊（東京大学）

生命現象の光操作技術の創出

13:35～14:00　　O-12 澤井　仁美（兵庫県立大）
環境変化に応じて生命を維持するための精密機械「センサータンパク質」の仕組みを探る

14:00～14:20　　休憩

【座長：前田　瑞夫】

14:20～14:55　　O-13 渡邉　力也（渡邉分子生理学研究室）
人工生体膜チップを利用した膜タンパク質の１分子生物物理学

14:55～15:20　　O-14 Rodtichoti Wannapob（前田バイオ工学研究室）
Development of electrochemical sensors and biosensors based on porous electrode and conducting polymer

15:20　　終わりに

ポスター発表（5 月 10 日 20:00~22:00）

P-01　RF トラップの原理を応用した超低速不安定核ビーム生成装置の開発 II
高峰　愛子（上野核分光研究室）

P-02　エレクトロスプレー・冷却イオントラップ法によるニコチン・水クラスターの赤外分光　－ 水和によるプロトン化サイトスイッチング
石内　俊一（東京工業大学）

P-03　光電子分光法によるフェロセン末端自己組織化単分子膜の電気二重層の構造評価
WONG Raymond (Kim 表面界面科学研究室)

P-04　Decay dynamics and diffusion properties of bright and dark excitons in air-suspended carbon nanotubes
石井　晃博（加藤ナノ量子フォトニクス研究室）

P-05　Application of heterodyne-detected vibrational sum frequency generation spectroscopy to electrode/electrolyte solution interface
佐山　篤（田原分子分光研究室）

P-06　界面選択的非線形分光計測
二本柳　聡史（田原分子分光研究室）

P-07　Transfer Matrix used in beam trajectory simulation for any ion optical elements
Mishra　Preeti Manjari (東原子分子物理研究室)

P-08　Atomic-scale exploration of the stepwise metal-incorporated cycloaddition reaction in two dimensions
Chi Zhang (張 弛) （Kim 表面界面科学研究室）

P-09　ミューオニウム原子超微細構造の精密分光による束縛系 QED の検証
上野恭裕（東原子分子研究室）

P-10　2 次元層状物質を用いた FET における界面特性に関する研究
方　楠(加藤ナノ量子フォトニクス研究室)

P-11　Investigation of Self-Assembled Triptycene Tripods on Ag(111) as Ultrathin Insulating Films by Scanning Tunneling Microscopy

Chaunchaiyakul Songpol（Kim 表面界面科学研究室）

P-12　二次元蛍光寿命相関分光法を用いた生体高分子ダイナミクスの研究
石井　邦彦（田原分子分光研究室）

P-13　ESR Method for Quantitative Evaluation of Reactive Oxygen Species (ROS) from Biological Samples
大島　勇吾（加藤分子物性研究室）

P-14　帯電状態の分子を用いた三重項励起子の選択的形成
木村 謙介（Kim 表面界面科学研究室）

P-15　量子もつれ光を用いた新規吸収分光法の開発
松﨑　維信（田原分子分光研究室）

P-16　大豆根粒菌由来酸素センサータンパク質 FixL の構造機能解析
鎌屋　美咲（兵庫県立大学大学院）

P-17　生体システムによる一酸化窒素分解の分子機構
當舎 武彦（RSC・生命系放射光利用システム開発チーム）

P-18　Towards Investigations of Pre-Cooled Ions Stored in the RICE Storage Ring Via Action Spectroscopy
CHARTKUNCHAND KIATTICHART（東原子分子物理研究室）

P-19　超流動ヘリウム中導入原子の周囲に形成されたバブルの緩和時間測定に向けて
竹内　由衣花（上野核分光研究室）

P-20　Tip-enhanced resonance Raman imaging of a single molecule
Rafael B. Jaculbia（Kim 表面界面科学研究室）

P-21　DNA 修飾ナノ粒子の非架橋型凝集を用いる生化学分析法
宝田　徹（前田バイオ工学研究室）

P-22　ディラク電子系の NMR
藤山 茂樹（加藤分子物性研究室）

P-23　K 中間子ビームを用いたΛ(1405)の研究

浅野　秀光（岩崎先端中間子研究室）

P-24　X 線結晶構造解析によるヘムセンサータンパク質の分子機構の解明
西永　惠(兵庫県立大学)

P-25　K^-ビームを用いた反 K 中間子原子核の生成
山我　拓巳（中間子科学研究室）

P-26　非対称ドナーが構築する Bilayer タイプ分子性導体の合成と電子物性
上辺 将士（加藤分子物性研究室）

P-27　ユーグレナの青色光応答と重力走性
尾笹　一成(前田バイオ工学研究室)

P-28　枯渇効果で見る DNA ナノ粒子の分散安定性と凝集機構
藤田　雅弘（前田バイオ工学研究室）

P-29　DNA-Functionalized Nanoparticles for Biosensing Applications
Surachada Chuaychob（前田バイオ工学研究室）

P-30　Cryogenic molecular dynamics explored in RICE and helium droplets
久間　晋（東原子分子物理研究室）

P-31　分子伝導体$EtMe_3P[Pd(dmit)_2]_2$に対する一軸圧効果と電界効果測定
南舘　孝亮（加藤分子物性研究室）

P-32　超伝導検出器 TES の中性分子質量分析応用
岡田 信二（東原子分子物理研究室）

P-33　不安定核のレーザー分光測定にむけたオフラインイオン源の開発
田島　美典（上野核分光研究室）

P-34　キラリティ制御によるスピン偏極電流の生成と制御
須田 理行（分子科学研究所）

P-35　水素分子の超低エネルギー電子衝突全断面積の測定
奥村　拓馬（東原子分子物理研究室）

P-36　High-resolution imaging of carbon nanotubes using a nonlinear excitonic process

大塚　慶吾（加藤ナノ量子フォトニクス研究室）

P-37　Real space interface charge transport between undoped and highly doped GaAs for terahertz application
Maria Herminia Balgos (Kim 表面界面科学研究室)

P-38　Fabrication and characterization of air-suspended carbon nanotube light emitting diode structures
寺嶋亘（加藤ナノ量子フォトニクス研究室）

P-39　入射核破砕反応を用いた励起状態核 ^{52m}Fe ビームの開発
川田敬太（上野核分光研究室）

P-40　中性原子ビームを用いた星間分子反応の実験研究
中野祐司（立教大学）

2019 年度

「物質階層原理研究」＆「ヘテロ界面研究」

研究報告会

2020 年 2 月 4 日（火）－5 日（水）

於　理化学研究所 鈴木梅太郎ホール

1 日目：2020 年 2 月 4 日（火）

13:30－13:40　概要説明（加藤 礼三）

【座長：加藤 礼三】

13:40－14:25　I-1　サブサイクル近接場による超高速電子操作
武田 淳（工学研究院／横浜国立大学）

14:25－14:55　O-1　局所界面におけるエネルギー移動・変換・散逸過程の理解
：単一分子発光計測・制御の新展開
金 有洙（Kim 表面界面科学研究室）

14:55－15:20　O-2　分子モーターを用いた再構成可能スピンフィルタ
山本 浩史（協奏分子システム研究センター／分子科学研究所）

15:20－15:35　休憩

【座長：金 有洙】

15:35－16:05　O-3　カーボンナノチューブにおける暗い励起子から明るい励起子への変換機構の解明
加藤 雄一郎（加藤ナノ量子フォトニクス研究室）

16:05－16:35　O-4　多軌道系分子性導体におけるディラック電子系の開発
加藤 礼三（加藤分子物性研究室）

16:35－17:20　I-2　Coordination Self-Assembly（配位駆動自己集合）
藤田 誠（工学系研究科／東京大学）

17:45－19:45　意見交換会（広沢クラブ）

2 日目：2020 年 2 月 5 日（水）

【座長：上野 秀樹】

9:15－10:00　I-3　^{229}Th 原子核極低エネルギー準位と高精度原子核時計への応用
吉見 彰洋（異分野基礎科学研究所／岡山大学）

10:00－10:30　O-5　エキゾチック原子分光による基礎物理検証
東 俊行（東原子分子物理研究室）

10:30－10:45　休憩

【座長：東 俊行】

10:45－11:15　O-6　RI・重イオンビームを用いた学際的開発研究
上野 秀樹（上野核分光研究室）

11:15－11:45　O-7　K中間子束縛核の世界
岩崎 雅彦（岩崎中間子科学研究室）

11:45－12:10　O-8　重いクォークを含むバリオン励起状態の研究
野海 博之（核物理研究センター／大阪大学）

12:10－13:35　昼食

【座長：田原 太平】

13:35－14:20　I-4　チャネルとポンプ：いのちを支える２つのイオン輸送
神取 秀樹（工学研究科／名古屋工業大学）

14:20－14:50　O-9　一酸化窒素還元酵素：構造ならび反応機構解析
城 宜嗣（生命理学研究科／兵庫県立大学）

14:50－15:15　O-10　イオン認識タンパク質バリノマイシンの冷却イオン分光
－認識機構へのボトムアップアプローチ
藤井 正明（化学生命科学研究所／東京工業大学）

15:15－15:30　休憩

【座長：金 有洙】

15:30－16:00　O-11　テラヘルツ核運動の実時間観測による化学結合生成ダイナミクスの追跡
田原 太平（田原分子分光研究室）

16:00－16:30　O-12　DNA 間相互作用に基づくナノ粒子の組織化と枯渇効果
前田 瑞夫（前田バイオ工学研究室）

16:30－16:40　閉会挨拶（小安 重夫 理事）

16:40－16:45　終わりに（金 有洙）


17:48

第 5 回 ExpRes Dojo 道場

— 測定を支える基本要素“Sample & Probe” —

A Joint Workshop of Pioneering Projects

“Fundamental Principles Underlying the Hierarchy of Matter: A Comprehensive Experimental Study”

「物質階層の原理を探求する統合的実験研究」&

“Heterogeneity at Materials Interfaces”「ヘテロ界面研究」

Date: January 14 (Tue.) 2020　15:00 - 17:00

Venue: RIBF Conference Room (2F)

15:00 - 16:00　数間 惠弥子（Kim 表面界面科学研究室）

走査トンネル顕微鏡による微小極限の光科学を実現するプラズモニック金属探針の開発

Development of plasmonic metal probes for the realization of ultimate spectroscopies and chemical reactions with a scanning tunneling microscope

近年、走査トンネル顕微鏡（STM）に光照射・検出を組み合わせた光 STM による新奇な計測手法開発の発展が目覚ましい。中でも、金や銀の STM 探針と基板の間に光照射することで励起できる局在表面プラズモンは、探針直下の物質のラマン信号や蛍光の増強、化学反応を誘起できることから注目を集めている。一方で、プラズモン共鳴の波長と強度は探針の先端形状に強く依存するにもかかわらず、従来の手法は探針形状の制御性と再現性に課題があった。本発表では、光 STM を用いた新奇な局所分光分析および反応解析を実現するための要素技術であるプラズモニック金属探針の開発について紹介する。

16:00 - 17:00　加藤 礼三（加藤分子物性研究室）

分子性固体の電子物性研究における試料合成

Sample preparation in studies of electronic properties of molecular solids

有機化合物や金属錯体等を構成成分とする分子性固体は、「分子」が物性発現の基本単位となっているのが特徴で、明快な電子構造を持ち低次元性や電子相関効果に基づく多様な電子物性を示す。分子の化学修飾によって電子物性を制御できるので化学合成が重要な役割を担う。物性測定データの質は、用いる試料の質・サイズ・形状等に大きく依存する。一般に、分子性化合物の結晶は、種々の外的刺激に弱く、また大きく成長させることが難しい。多くの場合、物性測定と試料合成は分業体制になっており、測定屋と合成屋とでは立場や文化が大きく異なり、両者の相互理解が良い結果を得るための重要な要素となる。これは言い換えると物理と化学の連携である。日本のこの研究領域における強みの一つはこの連携が比較的うまくいっている点にある。ここでは、物性測定用の試料を合成する立場から、試料合成の現場、測定屋と合成屋との連携において留意しなければならない問題点等について ongoing の実例を含めて紹介する。


ExpRes 道場
UCLA

（６）国際交流・若手育成など / International interaction・foster the team members

○ 国際交流・外国人研修生受け入れ実績 / International interaction, foreign trainees

・ 岩崎中間子科学研究室
IPA 7（韓国１、中国１、マレーシア２、インドネシア３）、
JRA 6（インドネシア 5、ベトナム１）

・ 上野核分光研究室
IPA 2（中国 1、ウズベキスタン 1）

・ 東原子分子物理研究室
IPA 1（フランス）

・ 田原分子分光研究室
実習生 2（インド、ドイツ）、訪問研究員 4（インド、中国、イギリス）

・ Kim 表面界面科学研究室
基礎科学特別研究員 4（フィリピン 1、中国 2、韓国 1）、訪問研究員 1（アメリカ）、
特別研究員 6（韓国 2、フィリピン 2、タイ 1、カナダ 1）、協力研究員 1（韓国）、
IPA 4（韓国 1、中国 2、フィリピン 1）、JRA 1（韓国）、実習生 1（韓国）、研修生 1（韓国）

・ 加藤分子物性研究室
IPA 1（フランス）、JRA 2（韓国 2）、訪問研究員 1（ポルトガル）

・ 前田バイオ工学研究室
基礎科学特別研究員 2（中国 1、韓国 1）、特別研究員 1（タイ）、訪問研究員 1（台湾）、
IPA 2（中国 1、タイ 1）、研修生 1（台湾）、客員研究員 1（中国）

・ 細胞制御学 II 研究室、兵庫県立大
非常勤研究員 1（イギリス）

・ 加藤ナノ量子フォトニクス研究室
訪問研究員 2（インドネシア、インド）、実習生 1（ドイツ）

・ 分子科学研究所山本グループ
インターンシップ生 6（タイ 4、フランス 1、インド 1）、総研大生 1（タイ）、訪問研究員 1（ロシア）

・ 東工大藤井研究室
準客員若手研究員 2（ドイツ・フランス）、客員研究員 1（オランダ）、
WRHI 特任教授 6（アメリカ、ドイツ、フランス 2、ギリシャ、オランダ）

・ 大阪大学核物理研究センター・J-PARC グループ
国際物理コースダブルディグリープログラム博士課程 1（カザフスタン）

○ 受賞 / Awards

1. S. Winarsih（岩崎中間子科学研究室・IPA）: RIKEN Exchange Meeting, Poster Prize（Student Section）
2. R. Ramadhan（岩崎中間子科学研究室・IPA）: RIKEN Summer School 2017, Poster Prize (in Physics）
3. F. Astuti（岩崎中間子科学研究室・JRA）: International Workshop on Organic Molecule Systems, Batu Feringgih, Malaysia 2017, Poster Prize

4. D. P. Sari（岩崎中間子科学研究室・客員研究員）: International Workshop on Organic Molecule Systems, Batu Feringgih, Malaysia 2017, Poster Prize
5. J. Angel（岩崎中間子科学研究室・JRA）: The 4th International Conference on Functional Materials Science 2018, Bali, Indonesia, Poster Prize
6. S. Winarsih（岩崎中間子科学研究室・IPA）: The 4th International Conference on Functional Materials Science 2018, Bali, Indonesia, Poster Prize
7. S. Winarsih（岩崎中間子科学研究室・IPA）: RIKEN Summer School 2019, Poster Prize（Best Presentation）
8. S. Winarsih（岩崎中間子科学研究室・IPA）: RIKEN Summer School 2019, Poster Prize（in Physics）
9. 岩崎 雅彦（岩崎中間子科学研究室・主任研究員）: 第 1 回理研梅峰賞（2019 年）
10. 西畑 洸希（上野核分光研究室・訪問研究員）: 第 24 回原子核談話会新人賞（2017 年 10 月）
11. 中野 祐司（東原子分子物理研究室・専任研究員）: 日本物理学会若手奨励賞（2018 年 3 月）
12. 田原 太平（田原分子分光研究室・主任研究員）: 日本分光学会賞（2017 年 5 月）
13. 倉持 光（田原分子分光研究室・研究員）: 日本分光学会奨励賞（2017 年 5 月）
14. 田原 進也（田原分子分光研究室・特別研究員）: 平成 29 年度日本分光学会年次講演会若手講演賞（2017 年 5 月）
15. 倉持 光（田原分子分光研究室・研究員）: 13th Femtochemistry Conference Most Surprizing Results Award（2017 年 8 月）
16. 田原 太平（田原分子分光研究室・主任研究員）: 第 8 回分子科学会賞（2017 年 9 月）
17. 長谷川 一途（田原分子分光研究室・研修生）: 第 11 回分子科学会優秀ポスター賞（2017 年 11 月）
18. 田原 太平（田原分子分光研究室・主任研究員）: Outstanding Contribution to Raman Spectroscopy（2018 年 3 月）
19. 倉持 光（田原分子分光研究室・研究員）: 日本化学会優秀講演賞（学術)（2018 年 4 月）
20. Mohammed Ahmed（田原分子分光研究室・特別研究員）: 26th International Conference on Raman Spectroscopy Best Poster Award（2018 年 8 月）
21. 坂口 美幸(田原分子分光研究室・特別研究員) : 日本生物物理学会若手奨励賞（2018 年 9 月）
22. 倉持 光（田原分子分光研究室・研究員）: PCCP Prize（2019 年 3 月）
23. 田原 進也（田原分子分光研究室・特別研究員）: 日本化学会 優秀講演賞（学術）（2019 年 4 月）
24. 田原 太平（田原分子分光研究室・主任研究員）: TRVS “Lifetime Achievement” Award（2019 年 9 月）
25. 田原 太平（田原分子分光研究室・主任研究員）: Mizushima Raman Lecture Award（2020 年 2 月）
26. 倉持 光（田原分子分光研究室・研究員）: 令和 2 年文部科学大臣表彰（若手科学賞）（2020 年 4 月）
27. 倉持 光（田原分子分光研究室・研究員）: 令和 2 年分子科学研究奨励森野基金（2020 年 8 月予定）
28. 今田 裕（Kim 表面界面科学研究室・研究員）：The 8th RIKEN Research Incentive Award（2017 年 3 月）.
29. 木村 謙介（Kim 表面界面科学研究室・研修生）：第 6 回 ナノスケール分子デバイス若手講演会講演優秀賞（2017 年 3 月）

30. 木村 謙介（Kim 表面界面科学研究室・研修生）：日本表面科学会講演奨励賞（スチューデント部門）（2017 年 5 月）
31. 今田 裕（Kim 表面界面科学研究室・研究員）：日本表面科学会講演奨励賞（若手研究者部門）（2017 年 5 月）
32. 木村 謙介（Kim 表面界面科学研究室・研修生）：日本化学会第 7 回 CSJ 化学フェスタ優秀ポスター賞（2017 年 10 月）
33. 木村 謙介（Kim 表面界面科学研究室・研修生）：第 7 回 ナノスケール分子デバイス若手講演会優秀講演賞（2018 年 1 月）
34. Emiko Kazuma（Kim 表面界面科学研究室・研究員）：Poster Award (Engineering Prize), SPDR and FPR program screening subcommittee in RIKEN（2018 年 1 月）
35. 金 有洙（Kim 表面界面科学研究室・主任研究員）：平成 30 年度科学技術分野の文部科学大臣表彰（2018 年 4 月）
36. 今田 裕（Kim 表面界面科学研究室・研究員）：理研梅峰賞（2018 年 6 月）
37. 金 有洙（Kim 表面界面科学研究室・主任研究員）、今田 裕（Kim 表面界面科学研究室・研究員）：日本学術振興会ナノプローブテクノロジー第 167 委員会ナノプローブテクノロジー賞（2018 年 7 月）
38. Emiko Kazuma（Kim 表面界面科学研究室・研究員）：ACSIN-14 & ICSPM26 Young Researcher Award（2018 年 10 月）
39. Chi Zhang（Kim 表面界面科学研究室・基礎科学特別研究員）：ACSIN-14 & ICSPM26 Young Researcher Award（2018 年 10 月）
40. 金 有洙（Kim 表面界面科学研究室・主任研究員）：日本化学会第 36 回学術賞（2019 年 3 月）
41. 今田 裕（Kim 表面界面科学研究室・研究員）：日本物理学会若手奨励賞（2019 年 3 月）
42. 數間 恵弥子（Kim 表面界面科学研究室・研究員）：The 10th RIKEN Research Incentive Award（2019 年 3 月）
43. 今井 みやび（Kim 表面界面科学研究室・研修生）：日本物理学会学生優秀発表賞（2019 年 3 月）
44. 今井 みやび（Kim 表面界面科学研究室・研修生）：第 8 回 ナノスケール分子デバイス若手講演会講演優秀賞（2019 年 3 月）
45. 木村 謙介（Kim 表面界面科学研究室・研修生）：日本表面真空学会講演奨励賞（スチューデント部門）（2019 年 5 月）
46. 數間 恵弥子（Kim 表面界面科学研究室・研究員）：平成 31 年度花王科学奨励賞（2019 年 6 月）
47. 今田 裕（Kim 表面界面科学研究室・研究員）、三輪 邦之（Kim 表面界面科学研究室・客員研究員）、今井 みやび（Kim 表面界面科学研究室・特別研究員）、河原 祥太（Kim 表面界面科学研究室・研修生）、木村 謙介（Kim 表面界面科学研究室・研修生）、金 有洙（Kim 表面界面科学研究室・主任研究員）：日本表面真空学会会誌賞（2019 年 10 月）
48. 今井 みやび（Kim 表面界面科学研究室・特別研究員）：ICSPM27 Poster Award（2019 年 12 月）
49. Shunji Yamamoto（Kim 表面界面科学研究室・基礎科学特別研究員）：Poster Award (Physics Prize), SPDR program screening subcommittee in RIKEN（2020 年 1 月）
50. 木村 謙介（Kim 表面界面科学研究室・研修生）：東京大学総長賞（2020 年 3 月）
51. 木村 謙介（Kim 表面界面科学研究室・研修生）：東京大学新領域創成科学研究科研究科長賞（2020 年 3 月）

52. 木村 謙介（Kim 表面界面科学研究室・研修生）：第 47 回応用物理学会講演奨励賞（2020 年 3 月）
53. 數間 恵弥子（Kim 表面界面科学研究室・研究員）：第 69 回日本化学会進歩賞（2020 年 3 月）
54. 加藤 礼三（加藤分子物性研究室・主任研究員）：第 8 回分子科学会賞（2017 年 9 月）
55. 磯野 貴之（加藤分子物性研究室・特別研究員）：日本物理学会若手奨励賞（2017 年 10 月）
56. 南舘 孝亮（加藤分子物性研究室・特別研究員）："ISCOM2019 Poster Award"（2019 年 9 月）
57. 王 国慶（前田バイオ工学研究室・基礎科学特別研究員）："NMS-XIII Excellent Poster Prize Award"（2017 年 10 月）
58. S. Chuaychob（前田バイオ工学研究室・IPA）, M. Fujita, and M. Maeda：第 40 回日本バイオマテリアル学会優秀研究ポスター賞（2018 年 11 月）
59. 土戸 優志（前田バイオ工学研究室・協力研究員）：日本分析化学会関東支部 2018 年度新世紀新人賞（2019 年 1 月）
60. 余 力（前田バイオ工学研究室・IPA）：第 68 回高分子学会年次大会優秀ポスター賞（2019 年 5 月）
61. S. Chuaychob（前田バイオ工学研究室・IPA）："RIKEN Summer School 2019 Poster Award : Chemistry Prize & Special Prize for Most Inclusive Presentation"（2019 年 10 月）
62. S. Chuaychob（前田バイオ工学研究室・IPA）："Trace Analysis and Biosensor International Symposium I：Best Poster Presentation"（2020 年 2 月）
63. Rahman MD Mahfuzur（兵庫県立大細胞制御学 II 講座・D2 学生）：2018 Student Research Achievement Award, 62nd Biophysical Society Meeting （2018 月 2 月）
64. Menega Ganasen（兵庫県立大細胞制御学 II 講座・D3 学生）：第 18 回日本蛋白質科学会年会ポスター賞（2018 年 6 月）
65. 澤井 仁美（兵庫県立大細胞制御学 II 講座・助教）：第 42 回日本鉄バイオサイエンス学会学術奨励賞（2018 年 9 月）
66. 武田 英恵（兵庫県立大細胞制御学 II 講座・D2 学生）：第 56 回日本生物物理学会年会学生発表賞（2018 年 9 月）
67. Menega Ganasen（兵庫県立大細胞制御学 II 講座・D3 学生）：第 91 回日本生化学会大会若手優秀発表賞（2018 年 9 月）
68. 武田 英恵（兵庫県立大細胞制御学 II 講座・D2 学生）：兵庫県立大　知の交流シンポジウム 2018 優秀ポスター賞（2018 年 9 月）
69. 武田 英恵（兵庫県立大細胞制御学 II 講座・D2 学生）：RIKEN Summer School 2018, Poster Award Chemistry Prize （2018 年 9 月）
70. 武田 英恵（兵庫県立大細胞制御学 II 講座・D3 学生）：15th International Symposium on Applied Bioinorganic Chemistry （奈良） Student Award、（2019 年 6 月）
71. 城 宜嗣（兵庫県立大細胞制御学 II 講座・教授）：錯体化学会貢献賞（2019 年 9 月）
72. 石井 晃博（加藤ナノ量子フォトニクス研究室・特別研究員）：理化学研究所第 10 回研究奨励賞（桜舞賞）（2019 年 3 月）
73. 須田 理行（分子科学研究所・助教）：文部科学大臣若手科学者賞（2018 年 4 月）
74. 山本 浩史（分子科学研究所・教授）：日本化学会学術賞（2019 年 3 月）
75. 山本 浩史（分子科学研究所・教授）：永井科学技術財団学術賞（2020 年 3 月）
76. 藤井 正明（藤井研究室・教授）： 第 9 回分子科学会学会賞（2018 年 9 月）

77. 田村 将人（藤井研究室・M2）：東京工業大学・大隅ジャーナル賞（2019 年 6 月）
78. 藤井 正明（藤井研究室・教授）：フンボルト賞（2019 年 6 月）
79. 石内 俊一（藤井研究室・准教授）：第 4 回分子科学国際学術賞（2019 年 9 月）
80. 大塚 玲美奈（藤井研究室・M2)：第 13 回分子科学会優秀講演賞（2019 年 10 月）
81. 田村 将人（藤井研究室・M2)：第 13 回分子科学会優秀ポスター賞（2019 年 10 月）
82. 田端 みずき（藤井研究室・M2)：第 13 回分子科学会優秀ポスター賞（2019 年 10 月）
83. Zhadyra Omar（大阪大学核物理研究センター・J-PARC グループ・大学院生）：ANPhA 3rd Prize（2018 年 8 月）
84. 赤石 貴也（大阪大学核物理研究センター・J-PARC グループ・大学院生、共同研究員）：ハドロンユーザー会修士論文賞（2019 年 3 月）
85. Zhadyra Omar（大阪大学核物理研究センター・J-PARC グループ・大学院生）：ANPhA 1st Prize（2019 年 9 月）
86. Zhadyra Omar（大阪大学核物理研究センター・J-PARC グループ・大学院生）：Hashimoto Prize（2019 年 9 月）

○人材の転出 / Promotion of young researchers

1. 橋本 直（岩崎中間子科学研究室・基礎特別研究員）：日本学術振興会・特別研究員（2017 年 4 月）
2. 神田 聡太郎（岩崎中間子科学研究室・基礎特別研究員）：高エネルギー加速器研究機構物質構造科学研究所・助教（2020 年 1 月）
3. 佐藤 智哉（上野核分光研究室・基礎科学特別研究員）：東工大理学院・助教（2019 年 4 月）
4. 西畑 洸希（上野核分光研究室・基礎科学特別研究員）：九大学理学研究院・助教（2019 年 10 月）
5. 市川 雄一（上野核分光研究室・専任研究員）：九大学理学研究院・准教授（2020 年 4 月）
6. 中野 祐司（東原子分子物理研究室・専任研究員）：立教大学理学部・准教授（2017 年 4 月）
7. 岡田 信二（東原子分子物理研究室・協力研究員）：中部大学工学部・准教授（2020 年 4 月）
8. Paul Bertier（東原子分子物理研究室・IPA）：Oxford 大学・PostDoc（2017 年 9 月）
9. 井上 賢一（田原分子分光研究室・基礎科学特別研究員）：東北大学大学院理学研究科・助教（2017 年 10 月）
10. 竹内 佐年（田原分子分光研究室・専任研究員）：兵庫県立大学理学部・教授（2018 年 3 月）
11. 浦島 周平（田原分子分光研究室・特別研究員）：東京理科大学理学部・助教（2018 年 3 月）
12. 田原 進也（田原分子分光研究室・特別研究員）：大阪大学大学院理学研究科・JSPS 特別研究員（2018 年 3 月）
13. 倉持 光（田原分子分光研究室・研究員）：分子科学研究所・准教授（2020 年 3 月）
14. Holly Walen（Kim 表面界面科学研究室・訪問研究員）：Space Dynamics Laboratory (US Government Research Agent)・Senior Scientist（2018 年 6 月）
15. Bo Yang（Kim 表面界面科学研究室・IPA）：Xijing Univ., China・Research Assistant Professor（2018 年 10 月）
16. 磯野 貴之（加藤分子物性研究室・特別研究員）：学習院大学理学部・助教（2018 年 6 月）
17. 川椙 義高（加藤分子物性研究室・研究員）：東邦大学理学部・講師（2019 年 4 月）
18. 南舘 孝亮（加藤分子物性研究室・特別研究員）：東京理科大学理学部・助教（2020 年 4 月）

19. 張 家禎（前田バイオ工学研究室・訪問研究員）: 台湾工業技術研究院・研究員（2018 年 4 月）
20. 王 国慶（前田バイオ工学研究室・基礎科学特別研究員）: 中国海洋大学・教授（2018 年 4 月）
21. 土戸 優志（前田バイオ工学研究室・協力研究員）: 早稲田大学先進理工学部・助教（2019 年 4 月）
22. Rahman MD Mahfuzur（兵庫県立大細胞制御学 II 講座・D2 学生）: Univ. Texas Southwestern Medical Center・ポスドク（2018 月 2 月）
23. Menega Ganasen（兵庫県立大細胞制御学 II 講座・D3 学生）: 東京大学医科学研究所・ポスドク（2018 年 12 月）
24. 田中 駿介（加藤ナノ量子フォトニクス研究室・特別研究員）: 東京大学物性研究所・助教（2018 年 6 月）
25. 須田 理行（分子科学研究所・助教）: 京都大学工学部・准教授（2020 年 4 月）
26. 宮崎 充彦（藤井研究室・特定准教授）: お茶の水女子大学基幹研究院自然科学系・准教授（2019 年 10 月）
27. 石内 俊一（藤井研究室・准教授）: 東京工業大学理学院・教授（2020 年 5 月）
28. 山我 拓巳（核物理研究センター・教務補佐員）: 理研岩崎先端中間子研究室・特別研究員（2018 年 4 月）
29. 小松 雄介（核物理研究センター・特任研究員）: KEK・助教（2018 年 10 月）
30. 高橋 智則（核物理研究センター・特任研究員）: 理研延與放射線研究室・協力研究員（2019 年 4 月）

（７）研究課題予算（運営交付金）/ Budget (Institutional funding)

物質階層原理

千円

事業年度 Fiscal year		2017	2018	2019
総額	研究費 Research	73,397	65,117	65,619
	人件費 Personnel	28,764	37,044	34,381
	計 Total	102,161	102,161	100,000
Reizo KATO (including common budget for the project)	研究費 Research	11,403	22,557	9,860
	人件費 Personnel	11,158	1,204	140
	計 Total	22,561	23,761	10,000
Masahiko IWASAKI	研究費 Research	5,600	2,109	8,099
	人件費 Personnel	0	3,891	3,901
	計 Total	5,600	6,000	12,000
Hideki UENO	研究費 Research	11,092	6,972	6,513
	人件費 Personnel	1,508	4,528	4,987
	計 Total	12,600	11,500	11,500
Toshiyuki AZUMA	研究費 Research	257	3,581	3,483
	人件費 Personnel	12,343	7,919	8,017
	計 Total	12,600	11,500	11,500
Yousoo KIM	研究費 Research	12,600	9,000	16,000
	人件費 Personnel	0	0	0
	計 Total	12,600	9,000	16,000
Tahei TAHARA	研究費 Research	8,845	2,043	1,284
	人件費 Personnel	3,755	9,457	10,216
	計 Total	12,600	11,500	11,500
Mizuo MAEDA	研究費 Research	12,600	4,699	10,056
	人件費 Personnel	0	6,801	1,444
	計 Total	12,600	11,500	11,500
Yoshitsugu SHIRO	研究費 Research	11,000	9,656	7,787
	人件費 Personnel	0	3,244	3,713
	計 Total	11,000	12,900	11,500
Hiroyuki NOUMI	研究費 Research	—	2,000	2,000
	人件費 Personnel	—	0	0
	計 Total	—	2,000	2,000
Masaaki FUJII	研究費 Research	—	2,500	537
	人件費 Personnel	—	0	1,963
	計 Total	—	2,500	2,500

ヘテロ界面

千円

事業年度 Fiscal year		2018	2019
総額	研究費 Research	68,821	61,859
	人件費 Personnel	46,383	48,141
	計 Total	115,204	110,000
Yousoo KIM (including common budget for the project)	研究費 Research	3,071	6,884
	人件費 Personnel	13,033	8,816
	計 Total	16,104	15,700
Masahiko IWASAKI	研究費 Research	8,086	5,770
	人件費 Personnel	4,514	5,530
	計 Total	12,600	11,300
Hideki UENO	研究費 Research	12,000	8,692
	人件費 Personnel	0	3,208
	計 Total	12,000	11,900
Toshiyuki AZUMA	研究費 Research	6,741	4,946
	人件費 Personnel	5,859	6,354
	計 Total	12,600	11,300
Reizo KATO	研究費 Research	2,907	11,300
	人件費 Personnel	7,193	0
	計 Total	10,100	11,300
Tahei TAHARA	研究費 Research	10,441	9,386
	人件費 Personnel	2,159	1,914
	計 Total	12,600	11,300
Mizuo MAEDA	研究費 Research	8,613	1,828
	人件費 Personnel	3,987	9,472
	計 Total	12,600	11,300
Yoshitsugu SHIRO	研究費 Research	7,447	4,832
	人件費 Personnel	4,553	7,768
	計 Total	12,000	12,600
Yuichiro KATO	研究費 Research	7,515	6,737
	人件費 Personnel	5,085	4,563
	計 Total	12,600	11,300
Hiroshi YAMAMOTO	研究費 Research	2,000	1,484
	人件費 Personnel	0	516
	計 Total	2,000	2,000

（８） 研究業績（件数のみ）

物質階層原理

事業年度 Fiscal year		2017	2018	2019
原著論文 Original papers	欧文 English	50	43	49
	和文 Japanese	0	0	0
解説・著書 Reviews and books	欧文 English	2	1	11
	和文 Japanese	6	8	8
口頭発表 Oral presentations	国際会議 International	88	99	88
	国内会議 Domestic	128	105	80
シンポジウム開催 Hosted symposium	国際会議 International	4	6	3
	国内会議 Domestic	8	7	8
特許出願 Patent application		0	0	1

ヘテロ界面

事業年度 Fiscal year		2018	2019
原著論文 Original papers	欧文 English	34	47
	和文 Japanese	0	0
解説・著書 Reviews and books	欧文 English	4	2
	和文 Japanese	3	6
口頭発表 Oral presentations	国際会議 International	42	50
	国内会議 Domestic	42	49
シンポジウム開催 Hosted symposium	国際会議 International	4	2
	国内会議 Domestic	3	5
特許出願 Patent application		0	3

Research Achievements and Future Prospects

物質階層原理

1. Interaction in matter

Strong Interaction study by K-mesons in nuclei and nuclear matter

Iwasaki group (hadron sub-group) is investigating meson property in nuclei to understand strong interaction and a diversity of quark/hadron many-body systems woven by the strong interaction. The newest observation at J-PARC reviled the existence of $K^{-}pp$ state. We are aiming at the detail study of the observed $K^{-}pp$ state for the confirmation, and extend our study to the kaonic nuclear bound state in light nuclei. We are presently working on several proposals to J-PARC for the kaonic nuclear study. To conduct these experiments, we need to establish a totally new 4π spectrometer at J-PARC, to drastically improve the efficiency. The detail design of the new spectrometer system is in progress.

岩崎グループ（ハドロンサブグループ）は、原子核中に K 中間子を埋め込むことで中間子原子核束縛状態を生成し、強い相互作用が織り成す多様な状態を研究している。極めて最近、J-PARC での実験でこれまでに観測されたことのない K 中間子束縛核$K^{-}pp$の発見に成功した。我々は、この成果に基づき、さらなる詳細研究により発見された状態の存在を確立させるとともに、軽い原子核中における K 中間子束縛核研究を目指した複数のプロポーザルを準備しつつある。また、これらの実験研究のためには、全立体角に対して感度のある新規スペクトロメータを制作する必要がある。このため、新規スペクトロメータの詳細設計を同時に進めている。

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(1) S. Ajimura et al., Physics Letters B **789** (2019) 620-625

Unique nuclear deformation phenomena predicted at proton-rich RIs and their nuclear *interactions*: System development of collinear laser spectroscopy applicable for high-energy RI beams

Ueno group is developing apparatus for collinear laser spectroscopy for proton-rich RIs in the vicinity of ^{80}Zr, which are expected to show anomalous deformation phenomena. The development of the main part of the offline system has been almost completed so far, where all isotope shifts were accurately reproduced in the scheme to excite the $5d\ ^2D_{5/2}$-$6p\ ^2P_{3/2}$ (614 nm) transition and observe the $6p\ ^2P_{3/2}$-$6s\ ^2S_{1/2}$ (455 nm) natural emission light for $^{134-138}$Ba+ ion beams approximately at 10 keV, depending on the natural isotope abundance ratio.

上野グループは主として特異変形を示すと期待される ^{80}Zr 及びその近傍の陽子過剰核を対象とした、コリニアレーザー核分光研究に向けた装置開発を行っている。ここまでオフラインでの装置開発を進め、天然同位体存在比に応じた $^{134-138}Ba^{+}$ に対し 10 kV に加速したイオンビームを用いて $5d\ ^2D_{5/2}$-$6p\ ^2P_{3/2}$（614 nm）の遷移を励起し、$6p\ ^2P_{3/2}$-$6s\ ^2S_{1/2}$（455 nm）の自然放出光を観測する方法で正確に同位体シフトを決定でき、装置の主要部分の開発はほぼ完了した。今後、仁科センターのミッション研究として進める SLOWRI システム [1] の開発と並行し、オンライン実験に向けた当該装置の更なる開発を行い、テスト実験を経て Zr 陽子過剰核での測定に着手する。

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(1) M. Wada, Nucl. Instrum. Methods Phys. Res. B **317**, 450 (2013).

Interactions of slow molecular ion and neutral species via induced dipole *interaction*

Interactions of negative muon and nucleus via Coulomb *interaction* including QED effect

Azuma group has been developing the devices for collision experiments combined with a cryogenic ion storage ring RICE and a neutral beam in order to conduct a low-energy collisions of ions and neutral particles on the ground. This collision reaction is dominated by Coulomb interaction due to induced dipole moment and it play an important role in chemical evolution in molecular clouds in space. We have constructed a neutral beam line using a negative ion source and a photo-exfoliation laser and succeeded in producing an intense neutral carbon beam. We plan to proceed with full-scale merging experiments using hydrocarbon molecular ions and the neutral carbon.

Azuma group also conducted precision spectroscopy experiments of characteristic muonic X-rays emitted from muonic atoms isolated in a vacuum using the high-intensity slow negative muon beam supplied at J-PARC. The aim is to verify the quantum electromagnetism (QED) effect in Coulomb interaction under a strong electric field by precision spectroscopy with a multi-element superconducting X-ray detector. We succeeded in measuring the contributing 2-5 eV QED effect with an accuracy of 0.1 eV or less for 6 keV muonic X-ray. We will further analyze this absolute accuracy and compare it with theory, and further develop measurements for other noble gas atoms.

東グループは、イオンと中性粒子の低エネルギー衝突を地上で実験研究するために、極低温イオン貯蔵リングと中性ビームの合流衝突実験の開発を進めてきた。この衝突反応は、**誘起双極子モーメントによるクーロン相互作用**に支配され、宇宙空間の分子雲での化学進化において重要な役割を果たす。今までに、負イオン源と光剥離レーザーによる中性ビームラインを構築し強力な中性炭素ビームの生成に成功した。今後、炭化水素分子イオンと中性炭素による本格的な合流実験に進展する予定である。

また、J-PARC において供給される高強度低速負ミュオンビームを利用して真空中に孤立したミュオン原子から放出される特性 X 線の精密分光実験を実施した。多素子超伝導 X 線検出器を導入した精密分光によって**強電場下のクーロン相互作用における量子電磁気学（QED）効果を検証す**る狙いであり、実際にミュオニック Ne 原子からの 6 keV の特定 X 線に寄与する 2-5eV の QED 効果を 0.1eV 以下の精度で測定することに成功した。今後、この絶対精度に関する解析を進めて理論と比較するとともに、さらに他の希ガス原子を対象とした測定を展開する。

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(1) S. Okada, T. Azuma. D.A. Bennett, P. Caradonna, W. B. Doriese, M.S. Durkin, J.W. Fowler, J.D. Gard. T. Hashimoto, R. Hayakawa, G.C. Hilton, Y. Ichinohe, P. Indelicato, T. Isobe, S. Kanda, M. Katsuragawa, N. Kawamura, Y. Kino, Y. Miyake, K.M. Morgan, K. Ninomiya, H. Noda, G.C. O'Neil, T. Okumura, C.D. Reintsema, D.R. Schmidt, K. Shimomura, P. Strasser, D.S. Swetz, T. Takahashi, S. Takeda, S. Takeshita, H. Tatsuno, Y. Ueno, J.N. Ullom, S.Watanabe, S. Yamada, J. Low. Temp. Phys., *submitted*.

(2) T. Okumura et.al *in preparation*.

Magnetic *interaction and excitation* study in matter by means of μSR

Iwasaki group (muon sub-group) is responsible for operation of RIKEN-RAL muon facility at Rutherford Appleton Laboratory in UK. One of the major objectives of the facility is to study the magnetic interaction by using various μSR technics. We are studying magnetic interactions and low energy excitation in molecular quantum spin liquid system with Kato(R) Group. Electron transfer integrals are estimated from the first principles calculation and compared to macroscopic electronic properties by μSR and magnetic susceptibility measurements. For such projects, we plan to modify measurement conditions to run the magnetic susceptibility measurement system for a long time without time break with the high-pressure and electric-field applications. We also plan to arrange setups for microscopic measurements by μSR, ESR and NMR to be performed in parallel to obtain complementary information effectively and timely.

岩崎グループは、英国 Rutherford Appleton 研究所と共同で、同研究所内に理研-RAL ミュオン実

験施設を運営しており、ミュオンを用いた研究を行っている。中でも、**μSR 法を用いた様々な物性研究**は同施設の重要な柱である。本プロジェクトでも、同施設を活用している。特に、加藤（礼）グループと協力して、有機分子性結晶における量子スピン液体のような特異な磁性状態の磁気相互作用や低エネルギー励起を研究している。第一原理計算とミュオンおよび磁化測定を組み合わせることによって、マクロな電子状態を解明することを計画している。この計画を遂行するために、磁化測定装置の長期にわたる連続運転が可能な環境を整備するとともに、圧力や電場印加などの特殊測定条件を組み入れる装置の改良を試みる。さらに、電子状態を微視的立場から解明するために、μSR・ESR と NMR を相補的かつタイムリーに同時並行できる環境を整えることを目指す。

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(1) I. Watanabe, International Conference on Magnetism and Its Application (IICMIA2019), Solo, Indonesia, 20-21 November 2019.

(2) K. Wang, P. Murahari, K. Yokoyama, J.S. Lord, F.L. Pratt, J. He, L Schulz, M Willis, J.E. Anthony, N.A. Morley, L. Nuccio, A. Misquitta, D.J. Dunstan, K. Shimomura, I. Watanabe, S Zhang, P. Heathcote, and A.J. Drew, "Temporal Mapping of Electrophilic Photochemical Reactions and Excitonic Processes with Carbon Specificity" Nature Materials, **16**, 467–473 (2017).

Fabrication of molecular assembly by intermolecular *interaction*

Kim group is designing and fabricating molecular assemblies with various functions by precisely controlling the balance between intermolecular interactions and molecule-substrate interactions on solid surfaces. In collaboration with organic synthesis groups, Kim group discovered novel surface chiralities of molecular assemblies with planar[1)] and upright[2)] molecules. Moreover, they successfully visualized the stepwise cycloaddition reaction pathways of aromatic organic molecules with a scanning tunneling microscope (STM).[3)] These findings provide not only a deeper insight into organic thin films with high structural integrity, but also a new way to tailor interfacial geometric and electronic structures. Further research toward the functional expression of molecular assemblies will be carried out based on more complex intermolecular interactions.

Kim グループは、分子間相互作用と分子-基板相互作用のバランスを精密に制御することにより、多様な機能を持つ単分子膜を開発している。Kim グループは、有機合成グループとの共同研究により、平面状 [1)]および直立した [2)]分子からなる単分子膜における**新しい表面キラリティー**を見出した。さらに、芳香族有機分子の表面付加環化反応経路を STM により可視化することに成功した [3)]。これらの知見は、高度な構造完全性を持つ有機薄膜の形成への深い洞察を与えるばかりでなく、有機物／金属の界面における分子ネットワークの幾何学構造や電子構造を制御するための新たな道筋を示すものである。今後、より複雑な分子間相互作用に基づいた分子集合体のさらなる機能発現に向けての研究を行っていく。

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Interactions between electrons in multi-orbital molecular conductors

Kato(R) group is investigating electronic states in multi-orbital molecular conductors based on metal-dithiolene complexes with a small HOMO-LUMO gap. In the case of the strongly dimerized system, it was revealed that the HOMO-LUMO interaction induces charge/spin heterogeneity associated with the valence bond formation and the Coulomb repulsion. [1,2)] The heterogeneity can contribute to exotic electronic

states including quantum spin liquid. The nature of the low-energy excitation of the molecular quantum spin liquid will be studied in collaboration with Iwasaki group (μSR).

Kato(R) group, collaborating with theoreticians (Kumamoto Univ. and Nagoya Univ.), found that metal-dithiolene complexes can provide a single-component molecular Dirac electron system.[3] The tight-binding model revealed the mechanism of the Dirac cone formation where the HOMO-LUMO interactions play an important role. Based on the obtained material design, this group continues to develop novel Dirac electron systems.

加藤（礼）グループは、HOMO と LUMO のエネルギー差が小さい金属ジチオレン錯体を用いて、多軌道系分子性導体の電子状態を研究している。分子が強く二量化した系では、**HOMO-LUMO 相互作用**が valence bond 形成やクーロン反発相互作用と連携して、**電荷やスピンの不均化**を誘起することを見出した[1,2]。この不均化は、量子スピン液体等のエキゾチックな電子状態の形成に関与している。今後は、岩崎グループ（μSR）と協力して、量子スピン液体の低エネルギー励起の性質を調べる予定である。また、加藤（礼）グループは、理論研究者（熊本大、名大）の協力の下、金属ジチオレン錯体が**単一成分分子性ディラック電子系**を形成することを見出した[3]。強結合近似模型を用いてその形成メカニズムを明らかにし、HOMO-LUMO 相互作用が重要な役割を果たしていることがわかった。今後、ここで得られた物質設計指針に基づき、新しいディラック電子系の探索を続ける。

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Bottom-up approach to *interaction* mechanism in molecular recognition

Fujii(M) group is investigating molecular recognition mechanism in biomolecular and supramolecular systems by gas phase laser spectroscopy. Functional subsets in the molecular systems such as receptor are isolated and its molecular complex with ligands is generated under low temperature isolated condition. The laser double resonance spectroscopy including IR lasers can reveal the structure of the complex. The structural variation by changing the ligands are discussed in terms of the molecular recognition. We have been applying this “bottom-up” approach to β_2-adrenaline receptor[1, 2], potassium channel[3, 4], and action mechanism of Li salt[5]. Collaboration with theory groups (Dr. K. Yagi, Prof. Y. Yuji in Riken, Prof. A. Kitao in Tokyo Tech and Prof. Sotiris Xantheas in PNNL and WRHI TokyoTech) are also important to determine the structural variations of these flexible molecules. The approach will be expanded to other adrenaline receptors, ion channels and ionophores. The effect of hydration on molecular recognition will also be studied.

藤井（正）グループは、気相レーザー分光を用いて生体分子および超分子の**分子認識機構**を研究している。これら分子システムの機能性部分を取り出し、極低温気相孤立状態でリガンド分子との分子間錯体を生成させる。赤外レーザーを含むレーザー二重共鳴分光法によりこれらの錯体の構造を明らかにする。リガンドを変えた場合のこのサブセットの構造変化を分子認識の観点から議論する。この「ボトムアップ」アプローチはβ_2－アドレナリン受容体、カリウムイオンチャネル、リチウム塩の薬理作用に対して適応してきた。これら柔らかな分子の構造変化を明らかにする上で理論グループ（理研・八木清／杉田有治 G、東工大・北尾彰朗、PNNL／東工大 WRHI・S. サンチャス）との共同研究は重要である。今後このアプローチを他のアドレナリン受容体、イオンチャネルやイオノフォアに適用していく。分子認識に対する水和効果も明らかにしていく予定である。

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Interaction of proteins with other molecules regulates biological functions

Shiro group is investigating protein-protein and domain-domain interaction in bacterial denitrification and oxygen sensing systems by using structural biological techniques. The studies are showing how important the interaction is in functions of the protein systems, and how the interaction regulates cellular function[1,2]. The techniques utilized in these work could apply to other interaction system such as protein-DNA in the sensor system and super-complex system. In addition, we will study dynamic structure of protein complexes controlled by such interaction in cellular system, by using *in cell* NMR technique.

城グループは、構造生物学的手法を用いて、脱窒系酵素群あるいは酸素センサーシステムをターゲットにした、**タンパク質−タンパク質間、タンパク質内のドメイン−ドメイン間の相互作用**の研究を行ってきた。これにより、生体物質間の相互作用がその機能発現においていかに重要であるか、さらには細胞機能をどのように制御しているのかを明らかにしてきた[1,2]。将来的には、この手法を他の生体物質間相互作用系（例えば、センサーシステムにおけるタンパク質−DNA 複合体など）に展開していくと同時に、より大きな超分子複合体をターゲットにすることが可能である。さらに、このような相互作用が細胞内におけるタンパク質の動的な構造にどのように影響を及ぼしているのかを *in cell* NMR 等の手法を使って明らかにする。

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Interactions between DNA molecules for directed self-assembly of nanoparticles

Maeda group is investigating self-assembly of DNA-modified nanoparticles. Exploiting molecular interactions emerging between surface-grafted DNAs has allowed directed assembly of structurally anisotropic gold nanorods and nanoplates[1] and structural changes of linear gold nanoparticle chains.[2,3] Significantly high anisotropy in self-assembled structures was achieved by aligning isotropic nanoparticles with a different colloidal stability in a defined order. Validity of this method will be further demonstrated by producing various nanostructures, of which physical and chemical properties are also the subject of future study.

To clarify the DNA–DNA interactions that are responsible for assembly, the attractive forces working between brush-like DNA monolayers were measured by using colloidal probe atomic force microscopy[4] and optical tweezers. Effects of types of terminal base pair and types of supporting electrolyte were studied in detail, thereby revealing π–π stacking interaction between DNA terminal base pairs. The research group will try to control the stacking interaction by external physical and chemical stimuli for dynamic nanoparticle assembly.

前田グループは、DNA 修飾ナノ粒子の自己組織化を研究している。粒子表面に固定された DNA の間に生じる相互作用を活用して、形状異方性の金ナノロッド・ナノプレートの配向制御[1]や、金

ナノ粒子の線状集合体の構造変換[2,3]を達成した。分散安定性の異なる等方性ナノ粒子を、順序を規定して配列し、その自己組織化において高い構造異方性が生じることを示した。今後は、集合構造の多様性を拡張して方法の妥当性を実証するとともに、集合体の特性評価を行う予定である。

その原理検証として、コロイドプローブ原子間力顕微鏡法[4]と光ピンセット法を用いて、DNA 単分子層の間に発現する引力を実測することにも成功した。末端塩基対の種類や支持電解質の影響を明らかにし、**DNA 末端近傍に生じる局所的な分子間相互作用**に関する知見を得た。今後は、物理的・化学的な外部刺激による DNA 末端間相互作用の可逆的な制御に取り組み、動的ナノ粒子集合体に応用する。

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2. Excitation in matter

Magnetic *hyperfine-excitation* of the ground state of muonic hydrogen atom for proton Zemach radius measurement.

Iwasaki group adopted the laser resonant excitation of the muonic hydrogen hyperfine states and the muon spin polarization detection as the key techniques. We already had progresses such as the efficient production of muonic hydrogen atoms in a low density hydrogen gas target as low as 0.05 STP and the measurement of the muon spin residual polarization and its holding time after muonic hydrogen formation. Concerning the laser development, we confirmed the generation of base laser light and are testing the wavelength conversion components. We plan further laser system tuning, doubling the laser system for higher power, and the laser cavity production. Then we will introduce the laser to a low temperature hydrogen target and carry out the laser resonance spectroscopy to determine the hyperfine splitting energy and the proton Zemach radius.

岩崎グループは、ミュオン水素原子を用いた**陽子 Zemach 半径**測定について、ミュオン水素原子超微細構造遷移のレーザー励起とミュオンスピン偏極測定を主要技術に据えて開発を進めている。すでに、常温 0.05 気圧の水素気体を標的とした効率的ミュオン水素原子生成、ミュオン水素原子生成過程でのミュオンスピン残留偏極測定、残留偏極を利用した偏極度保持時間測定などの成果を得ている。レーザー開発においては、基本波発生の確認、波長変換部の効率測定などが進んでいる。レーザーシステムのチューニング、レーザー2 重化による強度倍増、レーザーキャビティの開発を進めたうえで、低温水素標的と組み合わせてミュオン水素原子微細構造の共鳴励起波長探索を実施し、陽子半径の決定を行う予定である。

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Spectroscopic study of *excited baryons* (*quark-excitations* in baryon) with heavy quarks

Noumi group of RCNP, collaborating with Iwasaki group, is conducting a spectroscopic study of excited baryons with a heavy, charm quark. We will measure production rates and decay properties of excited charmed baryons systematically to deduce motions of a quark pair (diquark correlation) confined in a baryon. We have succeeded to develop a high-throughput, trigger-less data acquisition system with a high efficiency of almost 100%[1)], a beam counter with a time resolution of better than 50 ps[2)], scintillation fiber trackers improving a rate capability 10 times better[3)]. They are expected to work under a high event rate induced by a high-intensity pion beam of 30 Mega Hertz at a momentum of 20 GeV/c. We will develop particle identification detectors by means of time-of-flight and ring-imaging Cherenkov radiation.

野海（阪大 RCNP）グループは、岩崎グループ（hadron）と協力して、重いチャームクォークを含むバリオン励起状態の生成と崩壊を系統的に測定し、バリオン内部のクォーク対の運動（ダイクォーク相関）を解明する研究に取り組んでいる。当グループは、効率がほぼ 100%の高効率トリガレスデータ収集システム [1)]、50ps を切る高時間分解能のビーム計数器 [2)]、これまでの 10 倍以上高い応答のシンチレーションファイバー飛跡検出器 [3)]の開発にそれぞれ成功した。これらは、チャームバリオン生成に必要な毎秒 3000 万個に上る大強度の、運動量 20 GeV/c の π 中間子ビームによる高頻度の反応事象環境下で事象峻別性能を発揮する。今後は、飛行時間法やリングイメージングチェレンコフ検出器を用いた粒子識別装置の開発を進める。

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Anomalous shell structure and deformation in the *excitation* states of RIs far from the β-decay stability line as the manifestation of unveiled nuclear many body effects.

Ueno group has developed a new method to produce highly spin-aligned RI beams efficiently, by combining advantageous features of high-energy heavy-ion nuclear reactions with the momentum-dispersion matching technique of ion optics.[1] Based on this method, the group is conducting excited (isomeric)-state nuclear-moment measurement for very neutron-rich RIs. The group have so far successfully measured the magnetic dipole moments of isomeric states in ^{75}Cu[2] and ^{99}Zr,[3] and found that these nuclei have a characteristic shell structure and exhibit anomalous deformation phenomena. In the future, taking advantage of the method, the group will extend our observation to the nuclear electric quadrupole moments of ^{99}Zr and the nuclear moments of RIs around heavier and double-magic-number nucleus ^{132}Sn, to study the nuclear structure from our own microscopic point of view.

上野グループは、高エネルギー重イオン核反応の特性を利用し、更にイオン光学の運動量分散整合を組み合わせて独自に開発した高効率・高核スピン整列 RI ビーム生成法 [1]により、**超中性子過剰核の励起状態（準安定励起準位）の核電磁モーメント測定**を展開している。ここまで ^{75}Cu[2]や ^{99}Zr[3]の準安定励起準位の磁気双極子モーメントの測定に成功し、それらの核が特徴的な殻核構を有し特異な変形現象を示すことを明らかにした。今後更に当該手法の利用による研究を展開し、^{99}Zr の核電気四重極モーメントや、更に重い核二重魔法数核である ^{132}Sn 近傍での核電磁モーメント測定を進め、独自手法に基づく微視的立場からの核構造研究を行う。

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Slow energy dissipation dynamics of *excited* molecular ions isolated in vacuum through laser-induced action spectroscopy

Azuma group has been exploring the long timescale excitation and deexcitation dynamics of molecular ions isolated in a vacuum using the ion storage ring. By measuring fragments generated by tunable laser irradiation, we succeeded in acquiring high-resolution rovibrational spectra of linear triatomic molecular ions (N_2O^+) that exceeds conventional precision. Furthermore, by observing slow dynamics of the vibrational cooling process for each level in the timescale of seconds, we have identified the characteristic behavior in which different vibration modes are involved, and found the level population distribution apart from the Boltzmann distribution. In addition, we discovered that, in the laser-induced electron detachment process of diatomic negative molecular ions (Si_2^-), the rotational and vibrational structure appears even in the delayed electron detachment that occurs several tens of microseconds after laser irradiation. This is due to the fact that the Born-Oppenheimer approximation is extremely-weakly broken, which is a process that has been overlooked in the time domain of the conventional measurement. Recently, we also started experiments with diatomic molecular ion (CaH^+). This is of interest not only for the deexcitation dynamics of the rotational level reflecting the large dipole moment and its active level control by a laser, but also for the measurement of fundamental physical constants using the vibration level.

東グループは、極低温イオン貯蔵リングを利用して、真空中に孤立した分子イオンの長い時間領域における励起および脱励起ダイナミクスを探求してきた。直線３原子分子イオン(N_2O^+)のレーザー合流による生成解離種の測定によって従来の精度を超えた高分解能回転・振動スペクトルの取得に成功した。さらにそれぞれの準位ごとの**振動冷却過程の秒オーダーのダイナミクス**を明瞭に捉えることにより、複数の振動モードが関与している様相や励起準位分布が大きくボルツマン分布から離れた挙動を突き止めた。また、２原子分子イオン(Si_2^-)のレーザー誘起電子脱離過程において、レーザー照射後数10マイクロ秒という遅延脱離においても回転振動構造が顕著にあらわれることを発見した。これは**ボルン・オッペンハイマー近似が極めて弱く破れている**ことに起因しており、従来の観測時間領域では、全く見落とされていた過程である。さらに最近、2 原子分子イオン(CaH^+)の蓄積実験に着手した。大きな双極子モーメントを反映した回転準位の脱励起ダイナミクスやそのレーザーによるその能動的制御のみならず、振動レベルを利用した基礎物理定数の測定という観点から興味が持たれる。

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Excitations in femtosecond – millisecond structural dynamics of complex molecules

Tahara group studies femtosecond – nanosecond dynamics of photoreceptor proteins and photo-functional molecular assemblies using femtosecond time-resolved spectroscopy. In particular for biomolecules, this group clarified ultrafast structural dynamics of not only the chromophore of photoactive yellow proteins[1)] but also the protein part of retinal proteins[2)] using femtosecond Raman spectroscopy. This group is tackling clarification of the origin of highly inhomogeneous ultrafast dynamics of retinal proteins.

Tahara group studies microsecond – millisecond conformational dynamics of biomolecules using

two-dimensional fluorescence lifetime correlation spectroscopy (2D FLCS) developed in this group. This group studied cytochrome *c* and a riboswitch while developing a new method to perform 2D FLCS using only single dye-labelling.[3] While further investigating folding/unfolding dynamics of biomolecules, this group will develop new experimental/analysis methods extending the application of 2D FLCS.

田原グループは、フェムト秒ーナノ秒領域において、**光受容タンパク質と光機能性分子集合体の超高速ダイナミクス**を解明している。特に生体分子については、光活動性黄色蛋白質の発色団だけでなく[1]、レチナール蛋白質の蛋白部分の超高速変化[2]をフェムト秒時間分解ラマン分光によって明らかにした。今後、レチナール蛋白質の超高速ダイナミクスの**不均一性**の起源の解明に挑戦する。

田原グループは、マイクロ秒ーミリ秒領域では、独自に開発した**二次元蛍光寿命相関分光**（2D-FLCS）を用いて生体分子の構造ダイナミクスを研究している。シトクロム *c* とリボスイッチの構造変化を研究するとともに、単一色素標識のみで 2D-FLCS を行う新しい方法[3]を開発した。今後、生体分子の折り畳みダイナミクスの研究をさらに進め、また 2D-FLCS の原理に基づきその応用を広げる新たな計測・解析法の開発に取り組む。

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Excitation of a single molecule by localized surface plasmon

Kim group investigates the excitation of a single molecule by the localized surface plasmon (LSP) generated when light is applied to the tip of a scanning tunneling microscope (STM). The underlying mechanisms of the LSP-induced chemical reaction were clarified at the single-molecule[1-5]. Observations revealed that, when the orbital hybridization at the molecular interface is weak, the energy of the plasmon directly excites the molecule, while when the orbital hybridization is strong, the charge generated on the metal surface in the process of relaxation of the plasmon is generated to directly excite the molecule. By controlling the degree of orbital hybridization, it will be possible to control the light energy, reaction efficiency, and reaction mechanism required for the reaction, and it can be expected to contribute to the development of new photocatalysts.

Kim グループは、STM 探針への光照射により発生する局所表面プラズモンを分子の励起源として用い、**単一分子の化学反応メカニズム**の詳細を明らかにした[1-5]。その結果、分子と金属の界面における軌道混成が弱い場合には、プラズモンのエネルギーが直接分子を励起する反面、軌道混成が強い場合には、ラズモンが緩和する過程により金属表面で生成される電荷が分子を励起して、化学反応に導くことが明らかになった。今後、**分子と金属の界面における相互作用**を制御することで、反応に必要な光エネルギーや反応効率、さらには反応機構の制御が可能になると考えられることから、新しい光触媒の開発に貢献すると期待できる。

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Dynamics of nitric oxide in biological system examined using *excitation* of caged NO

Shiro group evaluated structures and electronic states of short-lived intermediates appeared in the catalytic reaction of nitric oxide reductase by combinational use of time-resolved spectroscopic techniques and caged NO[1]. So far, caged compounds have been generally utilized in the cellular biological research, but now its application will be expanded into other research fields such as in functional and dynamic-structural analysis of bio-molecules. The information thus obtained will be provided to theoretical studies of bio-molecules, e.g., quantum chemical studies of the electronic structures of short-lived intermediates and/or molecular dynamics simulation. In future, our group has much interest in developing new techniques in structural analysis of the short-lived intermediates, by combinational use of caged compounds, X-ray crystallography and/or cryogenic electro-microscopy.

城グループは、一酸化窒素還元酵素を研究対象にして、その酵素反応中に現れる短寿命反応中間体の構造・電子状態解析に、caged NO を使う時分割分光解析を開発した[1]。caged 化合物は今までは細胞生物学の分野で活用されてきたが、本研究により生体分子の機能解析、動的構造解析に使える事が示され、今後もその利用法は拡大すると思われる。このように得られた情報は、生体分子の理論的研究、すなわち短寿命反応中間体の電子状態解析や生体分子の分子動力学シミュレーションへと提供できる。将来的には、X 線結晶構造解析や低温電子顕微鏡との組み合わせで、短寿命反応中間体の分子構造を明らかにできる手法へと展開したい。

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ヘテロ界面

3. Heterogeneity at atomic-scale interfaces

Property change of external substances induced by impurity atoms, and conversely, structural changes that impurity atoms undergo: Toward application of *atomic-scale interface* to device technology

Ueno group is working on the following two theme for this subject: Development of a technique to control electrical conductivity of diamond by ion beam irradiation in collaboration with Kato(R) group, and direct observation of the time evolution of Stokes shifts for impurity atoms (Rb) introduced in a superfluid helium medium [1] in collaboration with Tahara group. In the former subject, it is known that superconductivity can be induced by high concentration boron doping based on the CVD method,[2] and the group is searching for the irradiation and annealing conditions to reproduce the superconductivity by the scheme of boron beam implantation. Unfortunately, the superconductivity has not been confirmed so far. The group will carry out high-temperature and high-pressure annealing by using high-purity artificial diamond in the next step. The group will eventually try nitrogen doping. In parallel, the group will also challenge other experiments related to the control of material functions by beam irradiation. In the latter subject, the picosecond pulsed Ti:Sa pump laser of the Tahara group was installed into the superfluid helium experiment system of the Ueno group, where the de-excited fluorescence of Rb was confirmed in the preparatory study. In the next step, the group will try to reduce the background due to stray light and start the measurement with the time-correlated single-photon counting method (TCSPC).

上野グループは、不純物原子が環境に与える変化及びその逆について、次の二つの課題に取り組んでいる：加藤（礼）グループとの共同研究によってイオンビーム照射によるダイヤモンドの電気伝導性制御技術の開発を、田原グループとの共同研究によって、超流動ヘリウム媒質中に導入された不純物原子（Rb）に生じるストークスシフトの時間発展の直接観測を目指している。前者は CVD 法による高濃度ホウ素ドープでは超伝導発現が見出されており [1]、これをビーム照射で再現するための照射及び試料のアニールの条件探索を行っている。残念ながらここまで超伝導の発現は確認されていないが、今後純度の高い人工ダイヤモンドを用いた照射を行い、高温高圧アニーリングを試みる。最終的には窒素ドープによる研究へと進めたい。並行し、ビーム照射による物質の機能制御の様々な課題にも取り組む。後者では田原グループのピコ秒 Ti:Sa 励起パルスレーザーを上野グループの超流動ヘリウムシステムに組み込み、準備研究にて Rb の脱励起蛍光を確認する所まで進展した。今後は散乱光等によるバックグラウンドの低減化を図り、時間相関単一光子計数法（TCSPC）による測定に着手する。

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Molecular approach to *heterogeneity* at the nano-scale superfluid *interface*

Azuma group has been developing a superfluid nanodroplet beam as a challenge in producing cryogenic molecular ions including large molecular systems. The helium droplet is a nano-size liquid of helium at a temperature of 0.4 K. After the realization of capturing a large neutral molecule into the droplet and its spectroscopic study, the current research focuses on ionization of the captured molecule. First, we prepared a neutral aniline molecule into the droplet by collision and showed that it was isolated and well stabilized inside the droplet, the superfluidity of which is an ideal cold environment for atoms and molecules. The measurement of the optical absorption band revealed that the access to the phonon excitation of the

surrounding superfluid helium was enabled via heterogeneity at the superfluid-molecule interface. Laser photoionization selectively caused the ionization of the dopant molecule because helium is transparent in up to the vacuum ultraviolet range. With the preferred advantage in readily controlling the number of molecules to be captured, an ultracold atomic and molecular cluster is generated in the droplet when many species are captured together in a single droplet and their binding energy is released by evaporation of helium atoms. Here, we showed that the ultracold aniline cluster was efficiently created by photoionization. The combination of the ion-containing droplet beam with our ion storage ring RICE is expected to offer molecular approach to finite-size superfluid dynamics.

東グループは、巨大分子までを含む極低温分子イオンビームへの挑戦として、超流動ヘリウムナノ液滴ビームの開発に取り組んできた。ヘリウム液滴は温度 0.4 K のナノサイズ液体ヘリウムである。我々の研究は、巨大ヘリウム液滴への大サイズ中性分子の取り込みとその分光からさらに進展し、現在、液滴内包分子のイオン化の段階へと到達している。まずヘリウム液滴に中性アニリン分子を衝突により捕捉し、超流動という理想的な極低温孤立環境中にアニリンが単離安定化されることを示した。その吸収バンドの測定から、**超流動と分子のヘテロ界面を通じて超流動体のフォノンが励起**されることを明らかにした。またレーザーを用いた光イオン化により選択的に内包分子のみをイオン化することに成功した。ヘリウム液滴への内包分子数は容易に制御でき、多数の分子が単一の液滴に捕捉された場合は、結合エネルギーを液滴表面のヘリウム原子の蒸発で取り除くことにより極低温クラスターを生成することも可能である。ここでは液滴内に中性アニリンクラスターをまず捕捉することにより、光イオン化法で**極低温クラスターイオンが効率よく生成**されることを発見した。このイオン内包液滴を極低温イオン貯蔵リング RICE と組み合わせることにより、分子スケールでの有限サイズ超流動ダイナミクスへの展開が期待される。

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4. Heterogeneity at molecular interfaces

Elucidations of *molecular interfaces* using phase-sensitive second-order nonlinear spectroscopy

Tahara group studies molecular interfaces using phase-sensitive heterodyne-detected vibrational sum frequency generation (HD-VSFG) spectroscopy which has been developed in this group. This group succeeded in obtaining vibrational spectra of the Stern and Gouy-Chapman layers of the silica/water interface and clarified water structure of the electric double layer.[1)] This group also developed the in-situ reference method to calibrate the phase and amplitude of the electric field of VSFG signal generated in the electrochemical interface, and succeeded in application of HD-VSFG to buried the electrode/liquid (Pt electrode/electrolyte solution) interface for the first time.[2)] Furthermore, Tahara group investigated the quadrupole mechanism of the VSFG process theoretically and experimentally, extending fundamental knowledge about how to interpret VSFG spectra beyond the ordinary dipole approximation.[3)] This group will further study buried interfaces including polymer/liquid, oxide/liquid and electrode/liquid interfaces, while developing new experimental methods for elucidating the molecular-level structure of various interfaces.

田原グループは、界面のみで発生する非線形信号光の位相と振幅を測定する**ヘテロダイン検出振動和周波発生（HD-VSFG）分光**を用いて分子界面を研究している。シリカ／水界面のシュテルン層とグイーチャップマン層の各々の振動スペクトルを得ることに成功し、**電気二重層の水構造**を明らかにした [1)]。また、埋もれた電極界面から発する VSFG 光の位相と振幅を校正する「その場参照法」を開発し、電極／液体界面（白金電極／電解質界面）の HD-VSFG 測定を初めて実現した [2)]。さらに、振振動和周波発生過程における四極子機構を理論、実験の両面から研究し、どのように VSFG スペ

クトルを解釈するべきかについて、従来の双極子近似を越えて基礎的理解を拡張した[3]。今後は、様々な界面の構造を分子レベルで解明するための新しい実験的方法を開発するとともに、ポリマー／液体界面、酸化物／液体界面、電極／液体界面等の埋もれた界面の研究をさらに進める。

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Development of novel spectroscopic methods for investigating *molecular interfaces*

Kim group has been developing novel spectroscopic methods based on a scanning tunneling microscope (STM) to investigate various kinds of molecular interfaces. Single-molecule emission and absorption spectroscopy[1] was developed to describe electronically excited states and exciton formation[2] of a single molecule on the carefully-designed ultrathin insulating films[3], which was also theoretically supported[4]. These technologies were further extended to visualize single-molecule resonance Raman effect under the STM tip[5]. Kim group also achieved a molecular-scale understanding of the electrical double layers in the electrochemical system by combining electrochemistry not only with photoemission spectroscopy[6] but also with STM-based Raman spectroscopy[7]. Electrochemical and redox properties of bio-interface systems, such as membrane proteins and DNA monolayers, will be investigated in collaboration with Shiro group and Maeda group.

Kim グループは、走査型トンネル顕微鏡（STM）に基づく新しい分光法を開発して、さまざまな種類の分子界面を研究している。単分子発光および吸収分光法を開発し[1]、絶縁超薄膜膜表面上[2]の単一分子の励起子形成[3]や電子励起状態の詳細を研究し、理論解析を行った[4]。これらの独自に開発した分光法に基づき、**単一分子共鳴ラマン効果の視覚化**に成功した[5]。Kim グループはまた、電気化学手法を光電子分光法[6]や STM ラマン分光法[7]と組み合わせることにより、**電極表面上の電気二重層の分子スケールの理解**が可能になった。今後、膜タンパク質や DNA 単分子膜などのバイオ界面における電気化学的特性と酸化還元特性について、城グループおよび前田グループとの共同研究を行っている。

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Singular *interfacial* phenomenon of DNA brush and its applications for biosensing

Maeda group has studied on interfacial phenomenon of DNA-functionalized nanoparticles, called non-crosslinking aggregation. On the basis of the experimental results, principally X-ray analysis, it was considered that the difference in entropic effect due to the flexibility and motion of DNA strands accounts for the DNA structural dependency of colloidal stability.[1] The non-crosslinking aggregation is not facilitated by the base stacking attraction between the blunt ends of dsDNA.

We have considered that the change in DNA structure is a key role for non-crosslinking aggregation. Other DNA conformational transitions could also induce the change of colloidal stability. G-quadruplex (G4) DNAs are an outstanding candidate because the conformational changes are expected to occur in response to binding with specific target molecules. We demonstrated that a hazardous molecule can be detected specifically using gold nanoparticles immobilized with a G4 DNA structure.[2] Nano-biosensor based on G4-functionalized nanoparticles could be a good candidate to apply in various applications, especially biosensor and medical diagnosis.

前田グループは、DNA 担持ナノ粒子が示す特異な界面現象（**非架橋凝集**）のメカニズム解明に向けた研究を展開している。X 線解析といった構造科学的知見を主とした実験事実に基づき、DNA 鎖の自由度や運動性によるエントロピー反発力（立体斥力）の差異が特異な界面現象を特徴付ける重要な因子であり、非架橋凝集は DNA 末端間のスタッキング相互作用に起因するものではないことが示された。

DNA の構造変化による自由度や運動性変化が重要な因子であるとすると、特定分子との結合による構造変化もまたコロイド分散安定性に大きな影響を及ぼすと考えられる。この考えに基づいた**DNA 担持ナノ粒子のバイオセンサー**の設計を進めている。その一環として、四重鎖 DNA で修飾したナノ粒子を作製し、低分子化合物を特異的に検出する系の構築に成功した。様々な物質検出を可能とする DNA 担持ナノ粒子の開発指針を与えるものである。

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Iron dynamics (reduction, transport and sensing) on biological membrane-protein *interface*

Shiro group has been studying the iron acquisition in human and pathogen, since iron is an essential element for all of life. Some membrane-integrated proteins play crucial roles for the iron transport into cell. Our targets were human ferric iron reductase, pathogenic heme importer and pathogenic heme sensor proteins. We successfully determined their crystal structures and, on the basis of their structural information, discussed their functions on the membrane interface in molecular level[1]. These studies provided structural basis of membrane-proteins for understanding the iron dynamics in biological system from molecular to cellular level. These strategy must be kept in near future. In addition, we are successful to determine the membrane-integrated enzyme, e.g., pathogenic nitric oxide reductase, by cryogenic electro-microscopy, which is now a powerful tool to investigate membrane-protein interfaces.

城グループは、生命現象において重要な働きをしている鉄に関して、**ヒトおよび病原菌による鉄の取込み現象**の研究をしている。鉄の取込みは細胞膜上に存在するいくつかの膜タンパク質が重要な働きをしているが、その中でヒトの鉄還元酵素、病原菌のヘム（鉄ポルフィリン錯体）の取込むポンプ、ヘム濃度センサータンパク質の結晶構造を明らかにし、膜界面でのこれらタンパク質の機能発現を議論してきた [1]。この結果は、いくつかの膜タンパク質が連環して機能する「生体内鉄動態」を、分子から細胞レベルに渡って理解できる基盤を提供できている。将来的にもこの方向を進展させていく。その研究において重要な膜タンパク質の構造解析に、X 線結晶構造解析だけでな

く低温電子顕微鏡法も取り入れていくための準備も進めている。すでに、髄膜炎菌の一酸化窒素還元酵素の低温電子顕微鏡構造解析に成功している[2, 3)]。

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5. Heterogeneity at device interfaces

Carbon nanotube *device interfaces*

Kato(Y) group investigates exciton properties in carbon nanotubes, where Coulomb interactions are strong because of limited screening. By developing a telecommunication wavelength time-resolved photoluminescence spectroscopy system, dark-to-bright exciton conversion mechanism has been elucidated[1)]. In addition, enhancement of single photon generation rate by using photonic crystals was demonstrated[2)] in a collaboration with Los Alamos National Lab in the U.S. The measurement system will be utilized to study excitonic effects within devices interfaces. Kato(Y) group is also working to clarify the effects of nanotube-molecule interfaces. Effects of air molecules have been characterized[3)], and in collaboration with the Kim group, organic molecule interfaces have also been examined[4)]. Novel photonic devices that utilize ion implantation will also be explored in a collaboration with Ueno Group.

加藤（雄）グループは、遮蔽効果が弱いためにクーロン相互作用が強く働くカーボンナノチューブにおける励起子物性とそのデバイス応用について研究している。通信波長帯の時間分解蛍光分光装置を立ち上げ、**暗い励起子から明るい励起子への変換機構**を明らかにしたほか、米国ロスアラモス研究所との共同研究によりフォトニック結晶を利用した**単一光子発生レートの増強**に成功した[1,2)]。今後、この測定系を利用してデバイス界面における励起子の挙動を調べる予定である。また、分子との界面に由来する効果についても調査を進めており、空気中の分子吸着の影響[3)]や金グループの協力を得て有機分子吸着の影響について明らかにしてきた[4)]。今後は上野グループと協力してイオン注入を活用した光デバイスの実証実験に取り組む予定である。

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Interactions of electrons at the device *interfaces*

Yamamoto group at IMS is investigating electronic states in two-dimensional organic Mott-insulators at the field-effect device interface. In Mott-insulators, the strong electron interaction provides various nontrivial properties such as superconductivity. In their study, field effect devices such as FETs (field effect transistors) and EDLTs (electric double layer transistors) comprising organic Mott-insulators could trigger metal-to-insulator or metal-to-superconductor transitions by controlling the interface carrier density. In addition, the strain from the device substrate could affect the bandwidth of the Mott-insulators to switch the

electronic phases.[1,2] The observed phase diagram is significantly doping asymmetric, which was theoretically analyzed in collaboration with Yunoki group (CEMS). The details of the three-dimensional phase diagram thus obtained and its relation to the underlying mechanism will be thoroughly investigated by combining data from different device configurations and materials as well as by performing theoretical analysis.

Yamamoto group also found that chiral molecules could provide reconfigurable spin filter.[3] The chirality-induced spin selectivity (CISS) effect was combined with chiral molecular motor, of which uni-directional motion was driven by light or heat, to show spin-polarization switching in a magnetoresistance device. Based on the CISS in single molecular levels, this group continues to extend the idea to crystalline bulk materials.

分子研山本グループは、電界効果デバイス界面における二次元有機モット絶縁体の電子状態を研究している。モット絶縁体においては電子間相互作用が、超伝導などの非自明な現象を引き起こす。同グループは、有機モット絶縁体を用いた FET (field effect transistor)や EDLT(electric double layer transistor)において、界面１分子層のキャリア密度を変調することによって、**金属絶縁体転移や超伝導転移を引き起こす**ことができた。加えて基板からの歪みによってバンド幅を制御することで、同様の相転移を引き起こすことにも成功した[1,2]。さらに、超伝導相の分布にドーピング非対称性を見出し、柚木グループ（CEMS）と理論的解析を行った。今後は、このようなデバイスによって得られる相図とその根底にあるメカニズムを解明するために、様々なデバイス構造と物質を検証し、理論的解析との比較をさらに進める予定である。

また、山本グループは、キラルな分子モーターを用いた**スピン偏極デバイス**を開発した[3]。分子モーターは光や熱によってそのキラリティを反転させるため、CISS（chirality-induced spin selectivity）効果を組み合わせることによって外部刺激によるスピン偏極のスイッチが可能となった。今後、CISS 効果をさらに拡張し、新しいスピントロニクスデバイスの探索を行う。

---

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Control of strongly correlated electrons at a molecular *device interface*

Properties of strongly correlated electron systems can show drastic changes (phase transition) by tuning the bandfilling and bandwidth. Kato(R) group studied basic properties of an electric-double-layer (EDLT) transistor using a molecular Mott insulator with an antiferromagnetic ground state in collaboration with Yamamoto group (IMS). Combination of the EDLT doping (bandfilling control) and substrate bending (bandwidth control) successfully led to observation of ambipolar superconductivity surrounding the Mott insulating state and non-Fermi-liquid behaviors in the normal state.[1,2] They also found possibilities of the control of the electronic state in a Mott insulator with a different ground state (Valence Bond Order).[3] The device technique developed in this project will be applied to various kinds of Mott insulating states including the quantum spin liquid.

強相関電子系では電子の密度（バンド占有率）と運動エネルギー（バンド幅）を変化させることによって電子状態を大きく変化させること（相転移）ができる。加藤（礼）グループは、分子研山本グループ（分子研）と共同で、この性質を利用した**強相関デバイス**の基礎物性を調べており、分子性モット絶縁体の反強磁性相に対し、電気二重層ドーピングと基板曲げひずみを利用して電子の密度と運動エネルギーを制御することにより、両極性超伝導や常伝導状態における非フェルミ液体的振舞いを見出した[1,2]。また、反強磁性とは異なる基底状態（Valence Bond Order）を持つモット絶縁体に対しても、同様の手法で電子状態を制御することが出来ることを示した[3]。今後は、この手法

をさらに他のタイプのモット絶縁状態（量子スピン液体等）に適用する予定である。

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Research Highlights

Research Category

	物質階層原理		ヘテロ界面		
Category	**1**	**2**	**3**	**4**	**5**
M. Iwasaki	○	○	○		
H. Ueno	◎	○	◎		
T. Azuma	○	◎	○		
Y. Kim	○	○	○	○	◎
R. Kato	○		○		○
T. Tahara		○	○	◎	
M. Maeda	○			○	
Y. Kato					○
Y. Shiro*	○	○		○	
M. Fujii*	○				
H. Yamamoto*					○
H. Noumi*		○			

* outside RIKEN　　◎ Sub-project leader

	Research category (Sub-group)
物質階層原理	1. Interaction in matter
	2. Excitation in matter
ヘテロ界面	3. Atomic-scale interfaces
	4. Molecular interfaces
	5. Device interfaces

[Category 1]

Exploring a diversity of quark/hadron many-body systems woven by the strong interaction

（強い相互作用が織りなす多様なクォーク/ハドロン多体系の探求）

Masahiko Iwasaki[1], Takumi Yamaga[1], Fuminori Sakuma[1], Hiroyuki Noumi[2], Yue Ma[1], Hidemitsu Asano[1], and for the J-PARC E15 Collaboration

[1] Meson Science Laboratory RIKEN, [2]Research Center for Nuclear Physics, Osaka University

Since the prediction of the π-meson by Yukawa, the long-standing question has been whether a mesonic nuclear bound state exists, *i.e.*, whether a meson forms a quantum state at an eigen-energy E_M $(= M_M c^2)$ below the energy of meson mass $m_M c^2$ without promptly vanishing in the nuclear media. If it exists, it means that a meson $(\bar{q}q)$ forms a quantum state where baryons (qqq) exist as particles in a nuclear medium. At the hadron level, those two are not exclusive by the Pauli principle, but both are composed of quarks by the strong interaction. By studying the mesonic nuclear bound state, one can have essential information to answer the key questions, *e.g.*, how light hadron masses are generated from ~*massless* particles: quarks (m_q ~few MeV/c^2) and gluons ($m_g = 0$), how the properties of these mesons change in the nuclear medium, how hadrons are confined in the nuclear media, and the equation-of-state in nuclear (or star) matter. Therefore, many mesons have been examined over the past century, to see whether a mesonic nuclear bound state exists below the mass threshold with a binding energy $B_M \equiv m_M c^2 - E_M$.

We conducted a search experiment using $K^- + {}^3\mathrm{He}$ reaction at kaon momentum 1 GeV/c, where the nucleon knock-out $K^- N \to \bar{K} n$ reactions $(\bar{K} = K^- \ or \ \bar{K}^0)$ have the maximum cross-section. If such a quantum state exists, the scattered quasi-free $\bar{K}$ could have low momentum (q) referring to the spectator nucleons (~*at-rest*) in ^{3}He, so the $\bar{K}$ may form a nuclear bound state via the $\bar{K} + NN \to \bar{K}NN$ reaction rather efficiently. As a result of the Λpn final-state analysis, we observed an event concentration in the Λp-invariant mass (M) spectrum near the $\bar{K}NN$ formation threshold[1]. This event concentration indicating possible existence of quasi-bound state (unstable bound state) and its decay as an intermediate state in the reaction, *i.e.*, $K^- + {}^3\mathrm{He} \to X + n$, and X (K^-pp in charge) $\to \Lambda p$.

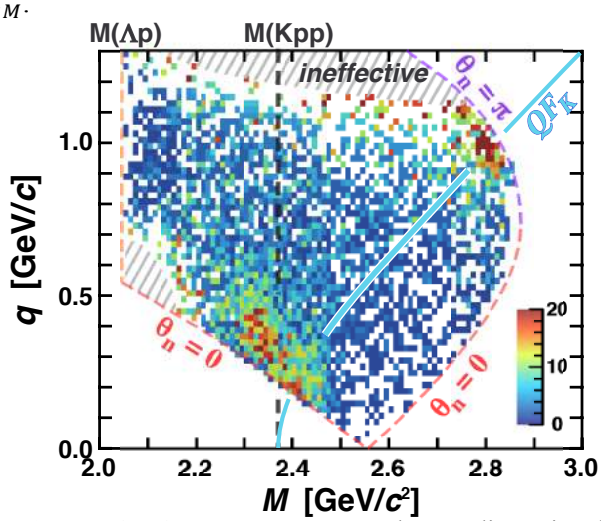

Figure 1. Acceptance corrected two-dimensional event distribution on momentum transfer (q) and Λp-invariant mass (M) of the Λpn final-state from the $K^- + {}^3\mathrm{He}$ reaction. Black dashed line indicates the mass threshold of $\bar{K}NN$ system and blue solid curve indicates the expected Λp-invariant mass coming from the on-shell kaon absorption reaction by the two spectator nucleons, $\bar{K} + NN \to \Lambda p$.

Fig. 1 shows the observed event distribution of the $K^- + {}^3\mathrm{He} \to \Lambda pn$ reaction measured by the Λp-pair over invariant mass (M) and momentum-transfer (q) plane[2,3]. We fitted the event distribution to represent that by the following three components, by simply formulated fitting functions; 1) K^-pp formation, the most distinct event-concentration located below the mass threshold of $\bar{K}NN$, and near the low q boundary, where K^-pp will be formed efficiently by emitting neutron at $\theta_n \approx 0$; 2) two-nucleon absorption of quasi-free kaon, $QF_{\bar{K}NN}$, a distribution around the blue-curve in the figure, where on-shell $\bar{K}$ absorption by two spectator nucleons, $\bar{K} + NN \to \Lambda p$, is expected; and 3) broad event distribution, distributing over whole kinematically allowed region having

relatively weak M and q dependence. The two event concentrations of component (2) at $\theta_n \approx 0$ and $\theta_n \approx \pi$ can be naturally understood as a kinematical reflection of Y^*(~1800) resonances, produced by the primary K^- momentum at 1 GeV/c ($\sqrt{s_{K^-N}} \sim 1.8$ GeV/c), having forward and backward peaking nature in $K^-N \to Y^* \to \bar{K}N$.

Figure 2 shows M and q spectra of the Λp-pair at the region of interest. In the figure, the fitted functions are plotted in red for the K^-pp formation (1), in blue for $QF_{\bar{K}NN}$ (2), and in green for the broad distribution (3). To our surprise, the fitted binding energy of K^-pp is as deep as ~ 40 MeV, while its decay-width is rather large ~90 MeV, so it is deep but quite unstable. There is another surprise, that the q distribution of K^-pp having much longer tail, whose gaussian form-factor parameter is deduced to be ~380 MeV/c, comparing to that of quasi-free kaon absorption. The long tail implies that the spatial size of K^-pp is as small as ~0.6 fm.

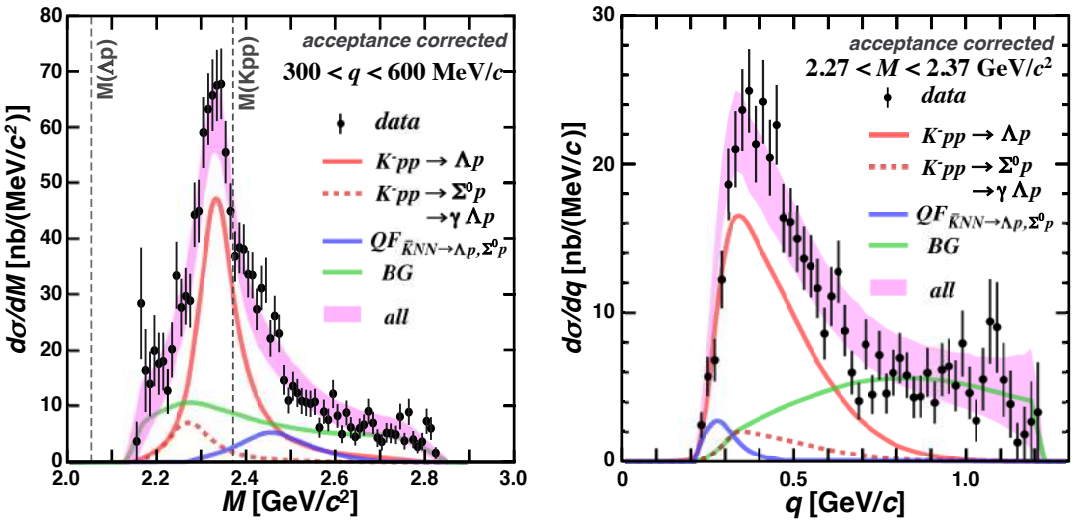

Figure 2. The Λp invariant-mass spectrum (left) and the momentum transfer spectrum (right) of the $K^- + {}^3$He reaction. The region of interest of the Λp-pair of the Λpn final-state are selected by q-slice for M spectrum (left) and by M-slice for q spectrum (right). Decompositions of the spectra are given in both figures.

We observed totally new form of nuclear system, K^-pp, which is composed by a boson and fermions in a hadron level, that had been looking for about a decade. The large binding energy indicating that the object is a tightly bound system, and the signal has long tail in form-factor function. Both facts are suggesting that the system could be extremely compact. All the hadrons are made of quarks, but confined as an individual particle even in nuclei, by the color-confinement mechanism of the strong interaction, but how is the question. We may access the fundamental key questions mentioned above in future from more detailed study of the system.

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[3] 岩崎雅彦、佐久間史典、山我拓巳, 日本物理学会誌、**855** 10 (2020)

意義と波及効果：中間子は原子核を構成する陽子・中性子（フェルミオン）を核中に繋ぎ止める核力の源（糊）として存在が予言されたボゾンである。一方で、中間子は陽子・中性子同様、強い相互作用によってクォークから構成され、核物質中では核力の支配下にあるハドロンの仲間である。データはK中間子が粒子状態（ハドロン）のままで2つの陽子と原子核状の量子状態を作りうることを初めて示した。クォーク多体型が如何に粒子としてのハドロンを生み、核物質中に在って尚、個別粒子として振る舞いうるかを調べることで、宇宙の成り立ちを紐解くことに役立つと期待される、基礎物理学研究全体に波及効果を持つ研究である。

[Category 1]

Unique nuclear deformation phenomena predicted at proton-rich RIs and their nuclear interactions: System development of collinear laser spectroscopy applicable for high-energy RI beams

（陽子過剰RI 領域独特の核変形現象とそれを生む核力：高エネルギーRI 用レーザー分光装置開発）

M. Tajima,[1] A. Takamine,[1] T. Asakawa,[3] M. Wada,[4] Y. Sasaki,[3] Y. Nakamura,[5] H. Iimura,[6,2] K. Okada,[7] T. Sonoda,[2] H. A. Schuessler,[8],∗1 H. Odashima,[4] Y. Matsuo,[3,1] and H. Ueno [1]

Nuclear Spectroscopy Laboratory, RIKEN,[1] SLOWRI Team, RIKEN Nishina Center,[2] Department of Advanced Sciences, Hosei University,[3] Wako Nuclear Science Center, KEK,[4] Department of Physics, Meiji University,[5] Nuclear Science and Engineering Research Center, JAEA,[6] Department of Physics, Sophia University,[7] Department of Physics and Astronomy, Texas A&M University [8]

Understanding of nuclear structure has so far been based on information obtained from stable nuclei. However, anomalous properties recently observed for unstable nuclei indicate unexplained part of many-body (collective) effects of the nuclear interaction, which have not yet been elucidated. In the present study, we focus on the proton-rich $N = Z$ nucleus $^{80}_{40}Zr_{40}$. This nucleus is theoretically expected to have well-developed deformation magic number 40 both in protons and neutrons, provided that the inversion of the $g_{9/2}$-$p_{1/2}$ single-particle levels takes place. Furthermore, such deformation will be largely enhanced by the realization of coherent action between protons and neutrons, and rich structures will arise from the coexistence/competition of different shape such as large quadrupole and tetrahedral shape deformations in or near the ground state, reflecting a significant change in the internal wave function. However, there are no experimental data on isotope shifts and nuclear moments, which we are interested in, because $^{80}_{40}Zr_{40}$ itself is difficult to produce and there are no experimental methods to match its low production yield and the short lifetime.

Collinear laser spectroscopy of RI beams is a powerful probe to directly measure the nuclear properties of ground or isomeric states. Thus, we have started the construction of the apparatus for collinear laser spectroscopy utilizing slow RI beams delivered from the SLOWRI system [2] of the RIBF facility. We designed and constructed an offline ion source for the planned optical spectroscopy of RI ion beams of refractory elements at a rate of 100 particle per seconds (pps). We note that zircon isotopes are available here, but not at most other RI beam facilities based on the ISOL (isotope separation on-line) method.

Figure 1(a) shows a schematic layout of the apparatus. The RF ion guide system composed of three segments of four SUS rods and an endcap. A solid target for laser ablation is fixed on the surface of the cylindrical electrode. Helium gas is introduced constantly and the typical pressure is approximately 22 mbar at the most upstream chamber. This ion source system is floated at 10 kV and connected to a test beamline through an insulation flange as shown in Fig. 1(b). The target is irradiated by an Nd:YAG laser pulse (532 nm, 10 ns width). First, the produced energetic ions are stopped via collisions with a He gas and guided to RF carpet system (RFCP) by a DC electric field. Then, the ions are subsequently guided to the downstream by RFCP, QPIG, and RFQ with applied RF and DC electric fields. After the ions are focused through the Einzel lens and four quadrupoles, they are separated depending on m/q using a dipole magnet and collected onto a Faraday cup (FC). Typical beam intensity at FC is 10^7–10^8 ions per laser pulse, which is sufficient for the demonstration of the planned spectroscopy of RI beams.

As a demonstration of collinear laser spectroscopy, we performed spectroscopy of barium ions, because barium is suitable for R&D study can be performed with an existing dye laser for one of the strong transitions $5d\ ^2D_{5/2}$-$6p\ ^2P_{3/2}$ (614 nm). A surface ionization source was constructed to obtain Ba^+ based on the design which was previously used at JAEA[3]. Barium oxide was heated up to approximately 2000 K and a few nA of Ba^+ were constantly produced. It was extracted at 10.5 keV, focused by electrostatic lenses, isotope-separated depending on m/q by a magnet, and focused again to enter an observation region. A CW dye laser (Coherent 899 Ring Laser) with Kiton Red pumped by a solid state laser (Verdi V10, 6 W) was irradiated collinearly with the Ba^+ beam. The power was 0.3 mW in the observation region. The FWHM of the laser frequency was 5 MHz. In the observation region, the velocity of ions was changed by using a set of electrodes. When the velocity was tuned according to the Doppler shift, the ion was on resonance and spontaneous emission from $6p\ ^2P_{3/2}$ to $6s\ ^2S_{1/2}$ (455 nm) successively occurred. This fluoresence signal was detected by a photomultiplier (Burle 8850). The quantum efficiency of the photomultiplier was about 20% at 455 nm, but the efficiency was less than 1% at 614 nm. Therefore, this measurement is almost free of background counts due to stray light of the laser. Figure 2 shows the counting rate of the fluoresence signal as a function of the applied voltage to the Doppler-shift-tuning electrodes. Isotope shifts and hyperfine splittings for $^{135,137}Ba^+$ whose nuclear spin $I = 3/2$ were successfully observed.

Trajectory simulations suggest that the resonance spectrum becomes asymmetric due to misalignment of the laser and ion beams, which can be a main systematic error. Detailed analysis is ongoing. We plan to introduce a fine tuning system of the alignment before the online measurement.

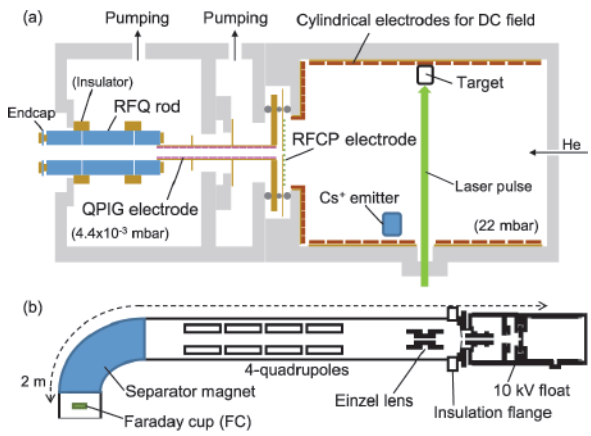

Figure 1 A schematic layout of (a) the ion-source system and (b) test beamline.

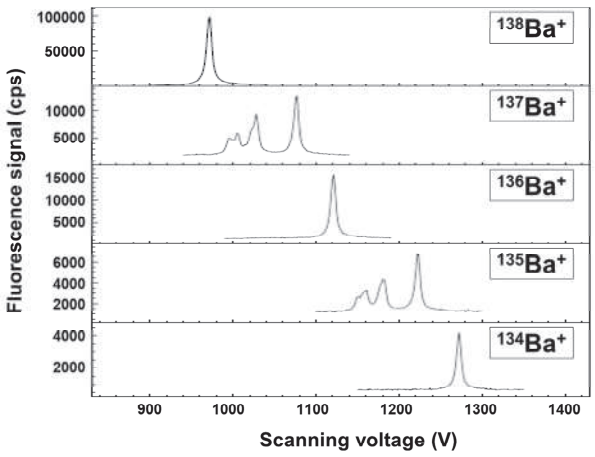

Figure 2 Resonance spectra for the isotopes $^{134-138}Ba$ transitions $5d\ ^2D_{5/2}$-$6p\ ^2P_{3/2}$.

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意義と波及効果：原子核は多様な性質を示す有限量子多体系である。研究が盛んに行われている中性子過剰核だけでなく陽子過剰核でも興味深い現象が理論的に予言されており、中でも Zr は Sn, Kr と並び、古くから注目されてきた特異変形を示す可能性がある注目の原子核であるが、実験技術的困難から測定が進んでいない。本研究は、RIBF+SLOWRI という独自の低速 RI ビーム生成様式と、本研究で開発しているレーザー分光装置を組み合わせることでこの状況を打破しようとするものである。この領域の特異変形に関する長年の議論に一石を投ずると共にレーザー核分光という RIBF の新たな利用展開を可能とする。

[Category 1]

High precision X-ray spectroscopy of muonic atoms for verifying QED under intense Coulomb interaction

（強クーロン相互作用下における QED 検証のためのミュオン原子精密 X 線分光）

T. Azuma[1], S.Okada[1], T.Okumura[1], S.Yamada[2] , T.Hashimoto[3] , P.Indelicato[4], Y. Miyake[5], T.Takahashi[6], D.S.Swetz[7], J. N. Ullom[7]

[1]AMO Physics Laboratory, RIKEN,

[2]Department of Physics, Tokyo Metropolitan University, [3]Japan Atomic Energy Agency (JAEA),

[4]Kastler Brossel Laboratory, Sorbonne University, and CNRS, France

[5] High Energy Accelerator Research Organization (KEK), [6]Kavli-IPMU,The University of Tokyo,

[7]National Institute of Standards and Technology (NIST), US

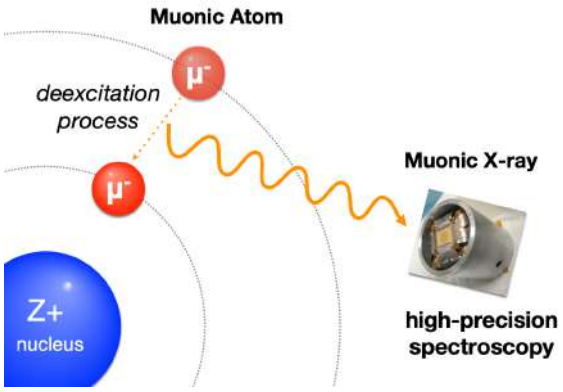

Figure 1 Schematic view of muonic atom and muonic x-rays

We performed the high-precision spectroscopy of muonic x-rays emitted from muonic atoms isolated in vacuum at J-PARC by introducing the superconducting TES detector. Negatively-charged muon with an intrinsic lifetime of 2.2 μs can be bound by the Coulomb field of an atomic nucleus. This system, so-called muonic atom, is a hydrogen-like exotic atom as schematically shown in Fig.1. The muon is about 200 times more massive than the electron. The Bohr radius is therefore 200 times smaller, and thus the internal electric field strength is to be 40,000 times higher than that of normal atoms. It is recently proposed that we can carefully choose X-ray transitions between the levels of relatively high principal quantum number and large angular momentum having significant quantum electrodynamics (QED) effect, but the nuclear size effect to them is negligibly small. This will provide a new horizon to explore the QED effect under extremely strong electric fields, which is a complimentary approach to the QED test using highly-charged heavy ions like U^{91+}. It is critical to prepare a low-density gas target (e.g., as low as 0.1 atom) to avoid the influence from the environment (for instance, electron transfer from the surrounding atoms). This condition was realized by the very-low-energy and high-intensity pulsed negative muon beam supplied at J-PARC. For high precision spectroscopy, we employed an X-ray spectrometer based on a multi-pixel array of superconducting transition-edge-sensor (TES) microcalorimeters. The 6.3 keV muonic X-rays for the 5g->4f and 5f->4d transitions of a Ne atom is one of the best targets for the measurement. The QED contribution of about 2-5 eV is expected for the transition and we have succeeded in verifying it with an accuracy less than 0.1 eV with the TES X-ray spectrometer to compare the state-of-art theoretical calculation.

The experiment was carried out at the D2 beam line of the muon facility MUSE (Muon Science Establishment) in the MLF (Materials and Life Science Experimental Facility) of J-PARC in April 2019 and January 2020. Typical intensity of the the negative muon beam is approximately $2x10^5$ cps at a momentum of 20 MeV/c. The beam was supplied by a double-structured pulsed mode with 25 Hz repetition rate. The incident muons were stopped in a Ne gas target (gas pressure of 0.1- 0.9 atm) where muonic Ne atoms were produced. X-

rays were emitted by the highly excited atoms and detected by a TES X-ray spectrometer.

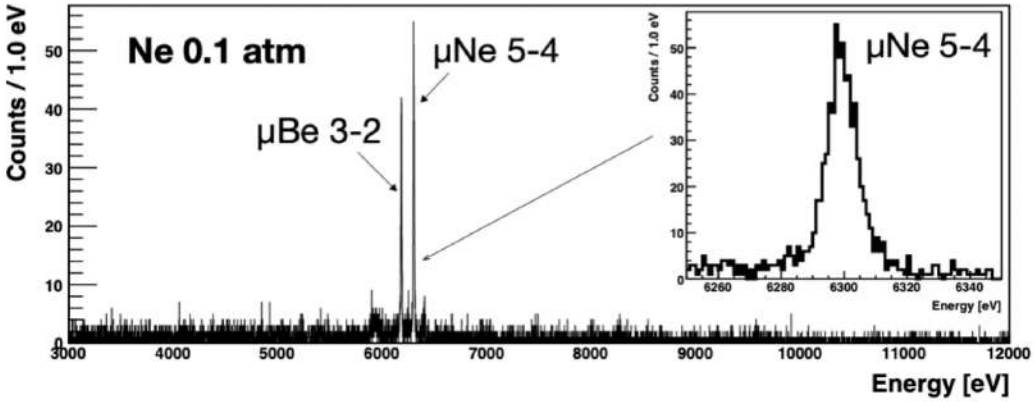

Figure 2 The detected muonic x-ray from the transitions of 5g-4f and 5f-4d. Note that a peak of μBe originates from the Be-foil window of the TES detector.

We employed an X-ray spectrometer based on 240-pixel TES array developed by the National Institute of Standards and Technology (NIST), US. Each TES pixel composed of a superconducting Mo/Cu proximity bilayer film having superconducting critical temperature of T_C~107 mK. A 4-mm-thick bismuth absorber is coupled to each TES to convert an incident X-ray energy to heat. The collimated effective area is 320μmx305μm for each pixel, and thus about 23mm^2 in total. This system is cooled with a pulse-tube-backed adiabatic demagnetization refrigerator (ADR). The regulated bath temperature was 70mK (~5mK rms). Each TES channel output was coupled to each individual first-stage SQUID amplifier.

Precise absolute energy calibration was critical for this measurement. Energy calibration during data acquisition was performed using characteristic K_α and K_β X-ray lines of Cr, Co and Cu using an X-ray generator by electron bombardment. Timing information was also used for rejecting the background signals. At around 6.30 keV, a clear time-energy correlation corresponding to muonic Ne 5->4 X-rays was successfully observed. The achieved energy resolution in the beam condition was concluded to be ~6 eV (FWHM) at 6.30 keV, which is evaluated to be enhough for enough an accuracy of 0.1 eV.

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[2] T. Okumura et al., *in preparation*.

意義と波及効果：負ミュオンが原子と衝突すると、負ミュオンは極めて高い励起状態に捕獲されたのち次々と脱励起し、負ミュオンと原子核のみから構成されるミュオン原子が生成される。この過程で負ミュオンは極めて原子核に近づいて核電荷に起因する強電場に晒されるため、ミュオン特性 X 線エネルギーの精密測定は、**強電場極限条件下での量子電磁力学 （QED） 相互作用を検証する**理想のプローブである。世界最高強度の超低速大強度負ミュオンビームを希薄ガス標的中に停止させることで、真空中に孤立ミュオン原子を用意し、多素子超伝導遷移端マイクロカロリメータ検出器によって、従来精度を遥かに凌駕するミュオン特性 X 線精密分光計測を実現した。高励起高角運動量準位間の遷移を測定することで、原子核の大きさに左右されることなく数 eV に及ぶ QED 効果を 0.1eV 以下の精度で決定することに初めて成功した。本プロジェクトのハドロン物理(岩崎研)と我々原子物理(東研)の研究者に加えて宇宙物理、加速器科学の研究者が連携することで達成した共同研究の成果は、基礎物理研究の新しい手法を提示したのみならず、広く他分野にブレークスルーとなる高精度 X 線観測手法を提供すると期待される。

[Category 1]

Nano-size effect on the La-based high-T_C superconducting oxides

— Abnormal modulation of the magnetic correlation at the boundary of CuO_2 planes —

（La 系銅酸化物高温超伝導体のナノ粒子効果

—CuO_2 面境界での磁気相関異常変調 —）

Isao Watanabe[1,2], Suci Winarsih[1], Redo Ramadhan[1], Irwan Ramli[1], Faisal Budiman[3], Hirofumi Tanaka[3], Takayuki Goto[4], Tadashi Adachi[4], Akihiro Koda[5]

Meson Science Laboratory RIKEN[1], Nuclear Spectroscopy Laboratory RIKEN[2],

Faculty of Engineering Kyushu Institute and Technilogy[3],

Department of Engineering and Applied Science Sophia University[4], Muon Group KEK[5]

Despite the fact that 30 years have passed since its discovery, high-temperature superconductors still contain many mysteries and are being studied from various perspectives. In the history of research conducted so far, efforts have always been made to synthesize fine, large single crystal samples. Such large-scale single crystals have enabled various studies and obtained a lot of information on the mechanism of high-temperature superconductivity and its antiferromagnetic correlation. In these discussions, it is premised that long-range magnetic correlation based on crystal continuity over the entire sample is realized, and conversely, most studies in which the magnetic correlation is spatially partitioned. Specifically, it is not obvious that the electronic state of the entire crystal changes when the magnetic correlation is broken at the layer boundary of the two-dimensional CuO_2 plane, which reflects the low-dimensionality of the La-based copper oxide crystal. This issue is an interesting research theme related to the essence of magnetic correlation that forms the basis of high-temperature superconductors. Such research themes are represented by thin film research by sputtering, but the problem of crystal distortion due to the difference in the structure of the crystal growth substrate and the structure of the crystal itself cannot be avoided, and the breakage of the

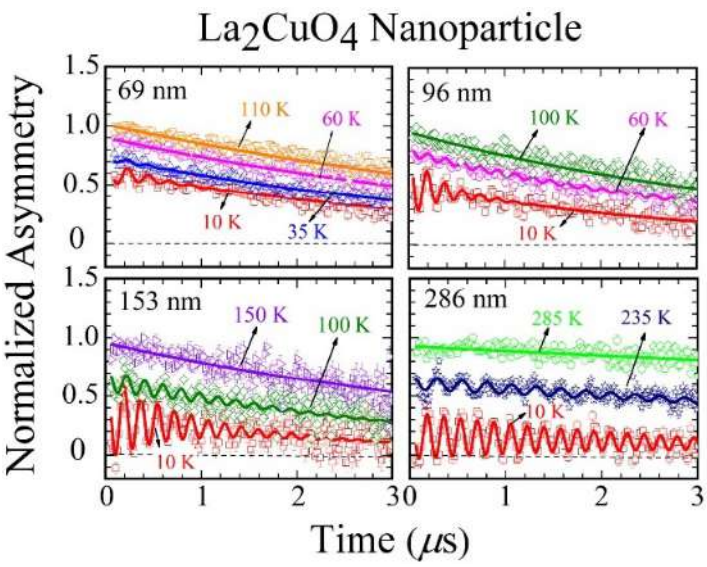

Figure 1 Zero-field μSR time spectra of four nano-particle samples of La_2CuO_4 measured at various temperatures. Sizes of nano particles are 69, 96, 153 and 286 nm determined by the X-ray diffraction measurement. The μSR experiments were carried out the RIKEN-RAL Muon Facility in the UK by using a pulsed muon beam.

magnetic correlation at the layer boundary is unavoidable. We have developed a high-temperature La-based copper oxide superconductor into nanoparticles, and created a magnetic correlation fracture surface at the interface between the surface (shell) and center (core) of the particles to change the electronic state. As research tools, magnetic measurements using a magnetic quantum meter and μSR, and particle size measurements using X-ray scattering and transmission electron spectroscopy were performed.

We synthesized four kinds of nanoparticles of La_2CuO_4 (LCO), which is a substance of La-based copper oxide high temperature superconductor, and identified the particle sizes as 69 nm, 96 nm, 153 nm and 286 nm, respectively. Figure 1 shows μSR time spectra measured in zero-field for each sample. LCO exhibits an antiferromagnetic transition at about 325 K in the bulk state and the spontaneous muon-spin rotation associated with antiferromagnetic alignment of copper spins is observed. As shown in Fig. 1, muon-spin precession was observed at low temperatures in each LCO sample. It was found that the ground state is an antiferromagnetically ordered state like the bulk state. The muon-spin precession amplitude becomes smaller as the particle size becomes smaller. Since the precession amplitude reflects the magnetic volume fraction of the antiferromagnetic ordered state, this result means that the region showing the antiferromagnetic ordered state decreases with the grain size.

The muon-spin precession frequency is the same as the rotation frequency in the ground state as observed in the bulk state. The muon-spin precession frequency corresponds to the spontaneous internal magnetic field at the muon position. The internal magnetic field also reflects the alignment of the magnetic moment of Cu surrounding the muons. That is, the magnitude and alignment of the magnetic moment of Cu in the antiferromagnetically ordered state in the nanoparticles are the same as in the bulk state.

It was also found that the precession amplitude decreased with increasing temperature but the frequency did not change significantly. This means that the magnetic structure in the magnetically ordered state does not change and only its volume fraction decreases with temperature. Surprisingly, it was found that reducing the size of LCO nanoparticles dramatically reduces the magnetic transition temperature at which the internal magnetic field becomes zero.

意義と波及効果：金属におけるナノ粒子効果は、バルク状態とは全く異なる新しい電子状態を引き起こす可能性を持つ。しかしながら、銅酸化物高温超伝導体に代表される Mott 絶縁体系物質におけるナノ粒子効果はほとんど研究されていない。本研究はそこに新しい突破口をつくることを可能にした。低次元性物質の磁気相関に対するナノ効果を詳細に研究した最初の例でもあり、幅広い応用研究を呼び起こす意義と波及効果を持つ

[Category 1,4]

Visualization of stepwise cycloaddition reaction pathways via intermolecular interaction on a metal surface

（金属表面上における分子間相互作用による環化付加反応経路の可視化）

Chi Zhang, Emiko Kazuma, and Yousoo Kim
Surface and Interface Science Laboratory, RIKEN

Dehalogenative cycloaddition reaction is a powerful strategy to generate new ring scaffolds with π-conjugated features on the surface[1-4], and thus holds great promise towards atomically precise electronic devices or nanomaterials. However, there are still uncertainties of the intermediate states involved in the overall reaction and lack of understanding of underlying mechanisms, which are practical obstacles to further precise design and optimization of the cycloaddition reaction products. In this study, we clarified a metal-mediated dehalogenative cycloaddition reaction pathway by visualizing the step-by-step evolution of stable local minima toward cycloaddition products in real space (Fig. 1).[5]

We chose the 2,3,6,7,10,11-hexabromotriphenylene (HBTP) molecule as the molecular precursor with threefold ortho-dibromo substitution for possible dehalogenative cycloaddition into two dimensions on Ag(111). Based on our stepwise annealing strategy and scanning tunneling microscopy (STM) observations, we captured stable local minima in the reaction pathway, i.e., intact HBTP, mono-debrominated HBTP radical (debr-HBTP), dominant organometallic dimer and minor debr2-HBTP diradical, two-dimensional (2D) organometallic network and final cycloaddition products.

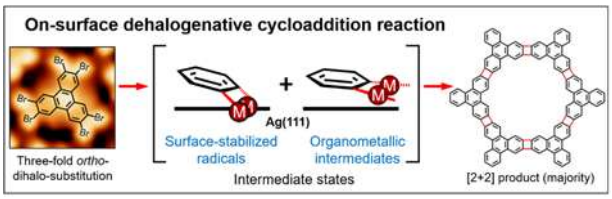

Fig. 1 Schematic illustration of the metal-mediated dehalogenative cycloaddition reaction pathway of HBTP molecule on Ag(111).

Based on the experimental observations, we further calculated the adsorption configurations of the molecular precursor, intermediate states, final covalent-bonded nanostructures, and the corresponding self-assembled structures on Ag(111). One typical intermediate state, that is, the 2D organometallic network structure, is shown in Fig. 2a as an example. Fig. 2a displays nice agreement between the experimental and theoretical results, further confirming the rationality of the hypothesis.

Finally, at higher temperature 2D covalent networks are formed after several competing intermediate states. Four elementary components, i.e., dominant di-TP, also cis-BTP and trans-BTP, and one minor tris-TP, are found to be involved in the covalent networks. Fig. 2b shows one covalent-bonded ring structure, which is constructed by the di-TP units via [2+2] cycloaddition reaction (Fig. 2c-e). The well-resolved phenyl rings indicate the direct correlation between the experimental results and the structural model, which provides good consistency in both dimensions and topography. Besides, the ability in the nice interpretation of long-range polymers based on the elementary components further provides solid evidence to support the assignment of different bonding modes.

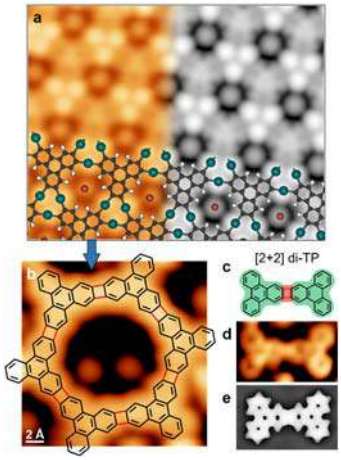

Fig. 2 (a) Submolecularly resolved STM image of the organometallic network (as one typical intermediate state) partially superimposed with the corresponding DFT simulation (the gray part) and structural model on Ag(111). (b) The STM image of one [2+2] ring structure superimposed with the chemical structure. (c) Chemical structure, (d) Submolecularly resolved STM image, and (e) Corresponding STM simulation of di-TP unit.

On the basis of the structural models, the climbing-image nudged

elastic band (CI-NEB) method has been used to find the transition states, and subsequently, the possible reaction pathways with the corresponding reaction barriers have been discovered (Fig. 3). Based on both experimental and theoretical indications, the underlying mechanisms of the on-surface dehalogenative cycloaddition reaction process have been revealed to provide an atomic-scale understanding of the overall reaction process.

As shown in Fig. 3, we revealed that the first process can be divided into three primary steps: Ⅰ. HBTP to debr-HBTP (debromination); Ⅱ. debr-HBTP to organometallic dimer (addition of adatom and radicals), and one side debromination step: Ⅱ'. debr-HBTP to debr2-HBTP; Ⅲ. organometallic dimer to trimer (addition of dimer and debr2-HBTP).

Fig. 3a shows the simplified energy diagram of the process (starting from HBTP, through debr-HBTP, and subsequently organometallic dimer and debr2-HBTP, toward organometallic trimer), in which the energy barriers of each process are provided along the reaction pathways. The typical reaction pathways involved and the corresponding structural models of the local minima (i.e., initial states (IS) and final states (FS)) and transition states (TS) are displayed in Fig. 3b-e. Such kinds of reaction pathways can be further extended to even larger areas forming 2D organometallic networks.

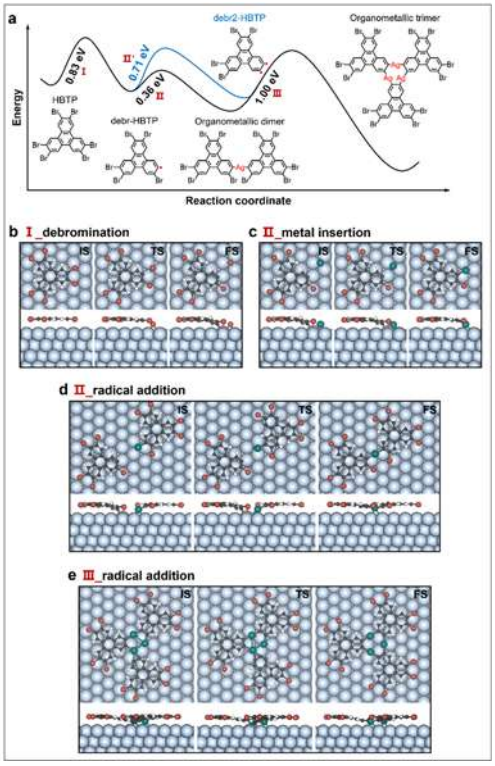

Fig. 3 DFT-calculated reaction pathways from intact HBTP toward formation of organometallic trimer on Ag(111). (a) Simplified energy diagram of the process. (b)-(e) Selected typical reaction pathways and the corresponding structural models of the local minima. (b) Debromination of HBTP to form debr-HBTP. (c) Metal insertion to debr-HBTP to form debr-HBTP+Ag. (d) Radical addition of debr-HBTP and debr-HBTP+Ag to form organometallic dimer. (e) Radical addition of debr2-dimer+2Ag and debr2-HBTP to form organometallic trimer.

As the final process, 2D organometallic networks convert to the dominant di-TP and very limited tris-TP units via formal [2+2] and [2+2+2] cycloadditions (cf. Fig. 2). The endothermic metal elimination process and exothermic cycloaddition process among unstable surface-stabilized radicals have further been revealed from the density functional theory (DFT) calculations.

In conclusion, we explored the on-surface stepwise metal-incorporated cycloaddition reaction experimentally and theoretically. This study clarifies the intermediate states involved where the metal serves as both platforms to stabilize the radicals and step-by-step participators in the organometallic intermediates. It also provides new mechanistic insights into the cycloaddition reaction, which has guiding significances for further precise design and optimization of the reaction products.

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意義と波及効果：金属表面上における分子間**相互作用**による段階的な金属含有環化付加の経路を、走査型トンネル顕微鏡を用いた実験と密度汎関数理論計算による理論計算に基づき明らかにした。表面安定化ラジカルと有機金属中間体の 0 次元から 2 次元への進化が、優位な共役四員環結合の形成に対して実空間で観察された。反応経路に基づいて、ラジカルと有機金属中間体の間の競合も解明された。これらの結果は、表面合成に関わる中間状態への基本的な洞察を提供するものである。

[Category 1]

Dirac electron system derived from HOMO-LUMO interactions in single-component molecular conductors

（HOMO-LUMO 相互作用が誘起する単一成分分子性ディラック電子系）

Reizo Kato[1], Hengbo Cui[1], Takao Tsumuraya[2], Takaaki Minamidate[1], Hamish H.-M. Yeung[3], and Yoshikazu Suzumura[4]

[1] Condensed Molecular Materials Laboratory RIKEN, [2] Priority Organization for Innovation and Excellence, Kumamoto University, [3] Inorganic Chemistry Laboratory, University of Oxford, [4]Department of Physics, Nagoya University

Molecular conductors have simple and clear electronic structures. This is mainly because only one kind of frontier molecular orbital (HOMO or LUMO) in each molecule contributes to the formation of a conduction band in conventional molecular conductors. In recent years, however, the number of molecular conductors that cannot be categorized to such a single-orbital system is increasing. This means that we should expand our perception toward a multi-orbital system where more than two molecular orbitals in the same molecule contribute to electronic properties and the orbital degree of freedom plays an essential role. A typical example of the multi-orbital system is single-component molecular conductor where the overlap of HOMO and LUMO bands generates conduction electrons. On the other hand, unusual electron transport properties of the Dirac electron system, where the occupied band contacts the unoccupied band at a point (Dirac point) with a linear dispersion relation in the wavenumber space (Dirac cone), has attracted a great deal of attention from theoretical and experimental viewpoints. A variety of materials with Dirac points in energy band structure have been developed. However, the number of systems where the Dirac point is located in the vicinity of Fermi level is still limited.

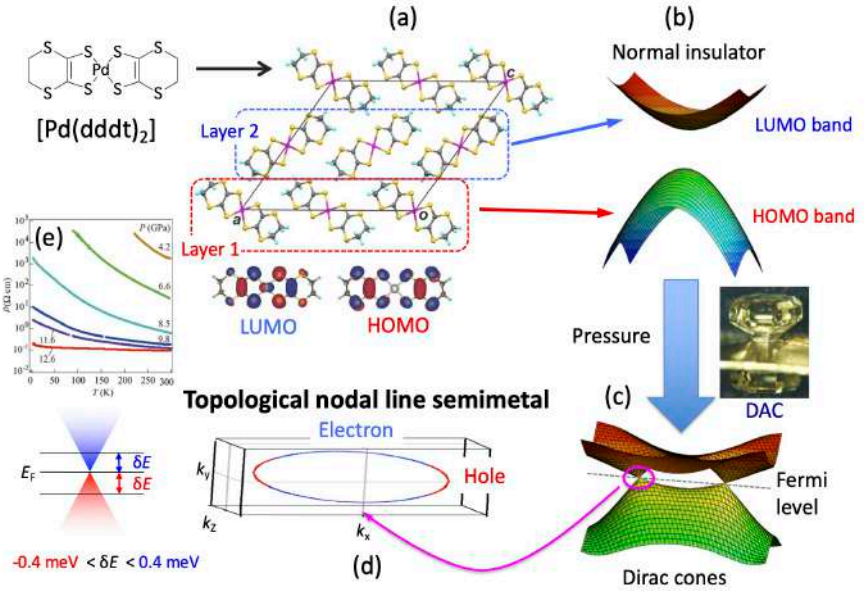
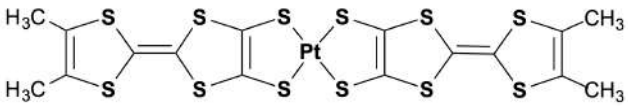


Figure 1 (a–e) Dirac cone formation in [Pd(dddt)$_2$] under high pressure. (a) Crystal structure of [Pd(dddt)$_2$] that consists of two crystallographically independent molecular layers. (b) Band structure that indicates a normal band insulating state under low pressure. (c) Dirac cones under high pressure generated by DAC. (d) The Dirac point describes a loop in the reciprocal lattice. A slight variation (±0.4 meV) of the energy from the Fermi level on the loop gives electron pockets and hole pockets. Such a system is called a topological nodal line semimetal. (e) Temperature dependence of resistivity under pressure.

We demonstrated that the Dirac electron system emerges in a single-component molecular conductor based on a metal dithiolene complex [Pd(dddt)$_2$] (dddt = 1,4-dithiin-2,3-dithiolate, Fig. 1(a)) under high

pressure.[1] The crystal of [Pd(dddt)$_2$] is an insulator at ambient pressure. The application of hydrostatic pressure using the diamond anvil cell (DAC) technique suppressed resistivity and activation energy. At 12.6 GPa, the resistivity hardly changes in almost all the temperature range (Fig. 1(e)). The first-principles density functional theory (DFT) calculations revealed that the Dirac cones are formed under pressure, which is consistent with the temperature-independent resistivity (zero-gap behavior). The Dirac cone formation in [Pd(dddt)$_2$] can be explained by a tight-binding model.[1–3] In the low pressure region, [Pd(dddt)$_2$] is a normal band insulator that includes fully occupied HOMO band and completely empty LUMO band with opposite curvatures (Fig. 1(b)). Since the metal dithiolene complexes with the square planar coordination geometry have a small HOMO-LUMO energy gap, enlargement of the bandwidth by the application of pressure can induce overlapping energy bands. Indeed, the HOMO band and the LUMO band overlap under pressure, which induces electron transfer from the HOMO band to the LUMO band. The Dirac point emerges when the HOMO and LUMO bands meet on the surface where HOMO-LUMO interactions are absent, that is, the gap formation does not work (Fig. 1(c)). The Dirac point is located near the Fermi level. This is a prominent feature of the single-component molecular system. The Dirac point forms a loop in the three-dimensional reciprocal lattice and its energy varies slightly from the Fermi level on the loop, which provides electron pockets and hole pockets. (Fig. 1(d)). This means that the system is a nodal line semimetal.

These results indicate that single-component molecular conductors can easily provide the Dirac electron system. Indeed, after our work, an ambient-pressure Dirac electron system based on a single-component molecular conductor [Pt(dmdt)$_2$] (dmdt = dimethyltetrathiafulvalenedithiolate) was disclosed by the first principles DFT band calculation.[4] We derived a tight-binding model for [Pt(dmdt)$_2$] and indicated that this system demonstrates a typical and simple example of the Dirac cone formation mechanism in the single-component molecular conductors, which promises the existence of next materials having similar electronic structures.[5]



[Pt(dmdt)$_2$]

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意義と波及効果：グラフェンに代表されるディラック電子系は、極めて動きやすい伝導電子をもち次世代エレクトロニクスへの応用が期待されているだけでなく、トポロジカル物質という新しい物質系探索への道を開いた。本研究は、単一成分の分子性結晶においてディラック電子系が形成されることを初めて示し、理論研究者との共同研究によって、その形成機構を明らかにして、フロンティア分子軌道である HOMO と LUMO に各々由来するバンド間に働く**相互作用**、分子軌道の対称性、分子配列等の役割を示した。これは、全く異なるカテゴリーに属するとこれまで考えられていた物質系（単一成分分子性導体とディラック電子系）が実は深く結びついていることを示すと同時に、分子性固体を用いたトポロジカル物質開発の指針を与えるものである。また、本研究において、ダイヤモンドアンビルセル（DAC）を用いた非常に高い圧力下での単結晶の電気抵抗測定技術が開発され、多くの共同研究が生まれている。

[Category 1,4]

Can the partial peptide SIVSF of the β_2-adrenergic receptor recognize chirality of the adrenaline neurotransmitter?

（β_2-アドレナリン受容体の部分ペプチド SIVSF は
アドレナリンのキラリティを認識できるのか？）

Masato Tamura,[1,2] Tsubasa Sekiguchi,[1,2] Shun-ichi Ishiuchi,[1,2] Anne Zehnacker-Rentien,[3,4] and Masaaki Fujii[1,2]

[11]Laboratory for Chemistry and Life Science, Institute of Innovative Research, Tokyo Institute of Technology, 4259, Nagatsuta-cho, Midori-ku, Yokohama, 226-8503, Japan

[2]School of Life Science and Technology, Tokyo Institute of Technology. 4259 Nagatsuta-cho, Midori-ku, Yokohama, Kanagawa, 226-8501, Japan.

[3]Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Univ. Paris-Sud, Université Paris-Saclay, F-91405 Orsay, France

[4]Tokyo Tech World Research Hub Initiative (WRHI), Institute of Innovation Research, Tokyo Institute of Technology, 4259, Nagatsuta-cho, Midori-ku, Yokohama, Japan

Chirality plays an essential role in biological molecular recognition, such as neurotransmission. However, data at the molecular level are scarce. X-ray crystal structures of active β_2-adrenergic receptors in interactions with their agonists are limited to agonists with natural chirality. Computer modelling and site-directed mutagenesis suggest that interactions involving β-OH located on the chiral carbon atom of adrenaline could be essential for achieving stereoselectivity.[1] Recent crystal structures of the agonist-bound β_2-adrenergic receptor reveal that recognition of the ligand involves a limited amino-acid sequence localized on the fifth transmembrane (TM-V) helix, namely SIVSF (S : serine, I : Isoleucine, V : Valine, F : phenylalanine).[2] This sequence acts as a binding site of the catecholamine agonists, with the two serine residues forming hydrogen bonds with the two catechol hydroxyls of the agonist.[2] These results prompted a gas-phase spectroscopic study concerning recognition of the partial CH_3CO-SIVSF-$NHCH_3$ peptide of the β_2-adrenergic receptor by proper (agonist) or non-proper neurotransmitters,[3] protonated like at physiological pH. Low-temperature gas-phase studies allow for the characterizing of molecular recognition without any conformational isomerism and multiple interaction sites. By combining a cryogenic ion trap (10K) equipped with an electrospray ionization (ESI) source with conformer-selective laser spectroscopy, we evidenced different binding patterns between SIVSF and proper or non-proper ligands.[3] While proper ligands, such as

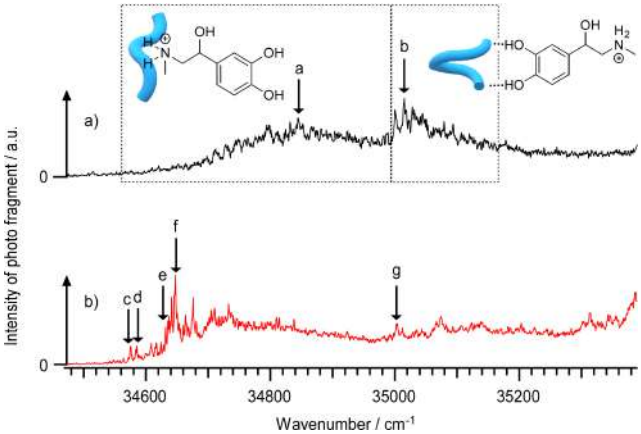

Figure 1 UV spectra of complexes of the SIVSF peptide with a) L-AdH^{+6} and b) D-AdH^{+} measured by UVPD spectroscopy which detects the photofragment m/z 607. Arrows and letters a-g indicate the bands probed by the

protonated L-adrenaline (L-AdH$^+$, see Figure 1b), form both catechol-bound and amino-bound complexes with SIVSF, only the amino-bound complex is observed for non-proper catecholamines ligands (noradrenaline and dopamine), although both ligands have catechol ring. Moreover, SIVSF adopts an α-turn structure, i.e. the shape of the TM-V helix under natural conditions, in catechol-bound complexes as well as the SIVSF monomer.[3] From an X-ray structural analysis, the SIVSF motif is thought to interact with the catechol ring only; however, results have revealed that SIVSF identifies the difference of amine chains. In this work, we interrogated the effect of chirality on the recognition process by comparing the structures of SIVSF-(L-AdH$^+$) and SIVSF-(D-AdH$^+$) complexes.

The UV spectrum of the SIVSF-AdH$^+$ complex changed drastically when L-AdH$^+$ was replaced by its enantiomer (Figure 1). The isomer-selected IR spectra shown in Figure 2 revealed that D-AdH$^+$ was bound to SIVSF by its protonated amino-group or a single catechol OH, and induced non-helical secondary structures of SIVSF. This is in sharp contrast to the helical SIVSF complex with L-AdH$^+$, which is close to the natural binding structure with two catechol OHs binding in the receptor. This shows that a short pentapeptide SIVSF can distinguish the chirality of the ligand AdH$^+$ as well as the receptor. This stereoselectivity is suggested to arise from an additional interaction involving the hydroxyl group on the chiral carbon. (Published as a cover paper of JPCL[4])

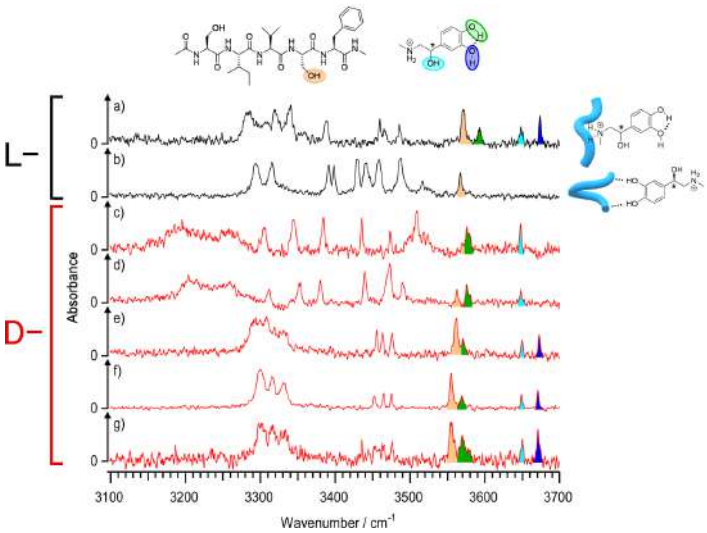

Figure 2 Isomer-selected IR spectra measured by IR-UV ion dip spectroscopy when the UV laser frequency was fixed to the bands at a and b of L-AdH$^+$ complexes, and c ~ g of D-AdH$^+$ complexes in the UV spectra (see Figure 1).

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意義と波及効果：キラリティは生体における分子認識で極めて重要な役割を果たしている。しかし、なぜ一方の光学異性体だけが認識されるのか、明確に分子レベルで示した例は極めて少ない。本研究はβ$_2$ーアドレナリン受容体の分子認識部位である部分ペプチド SIVSF に注目し、これに L—および D－アドレナリン分子を結合させ、それによるペプチドの構造変化を低温イオントラップレーザー紫外および赤外分光法で解明した。SIVSF は錯体形成するリガンドが受容体に認識されるか否かを構造に反映させることがわかっている。これにより、L—異性体と結合した SIVSF は受容体内と同じαヘリックス構造をとるが、D－異性体を結合した場合はヘリックス構造が取れないことがわかった。受容体のキラリティ認識が局所構造に由来することが明確に示され、創薬にも資する生体分子認識の分子論的学理が得られた。

[Category 1]

Interaction of Proteins with Other Molecules Regulates Biological Functions

（タンパク質相互作用による生理的機能の制御）

Yoshitsugu Shiro[1], Hitomi Sawai[1], Takehiko Tosha[2], Yasuhiro Koteishi[1], and Hiroshi Sugimoto[2]
[1]Cellular Regulation Laboratory, University of Hyogo, [2]RIKEN RSC

Interaction of a protein with other molecules, e.g., other proteins, is essential process to regulate cellular function in living system. Hydrophobic, electrostatic, hydrogen-binding and van der Waals interaction promote formation of protein-protein complex, and molecule(s), group(s) or ion(s) can be transferred from one protein to others as a signal or substrates for next catalytic steps. In our study, we have utilized structural biological techniques such as X-ray crystallographic and small angle X-ray scattering techniques for characterization of such interaction in the complex. Our targets were enzymes involved in bacterial denitrification process, and proteins in bacterial oxygen (O_2) sensor system.

1. Complex of Nitic Oxide Reductase and Nitrite Reductase

Denitrification is one of an anaerobic respiration system of microorganisms, in which nitrate (NO_3^-) and nitrite (NO_2^-) ions are converted into dinitrogen gas (N_2), through an intermediate formation of nitric oxide (NO) and nitrous oxide (N_2O). The denitrification is a part of the important process in the global nitrogen cycle, and consists of four reaction steps, all of which are catalyzed by four metal-binding enzymes. On intermediate, NO, is produced in one-electron reduction reaction catalyzed by Fe-containing Nitrite Reductase (NiR): $NO_2^- + e^- + H^+ \rightarrow NO + H_2O$. NO thus generated is a radical molecule, and exhibits a high cyto-toxicity, usually leading a cell death. However, the denitrification microorganisms can survive under denitrification condition, because it is decomposed into non-toxic N_2O (detoxification) in the two-electrons reduction reaction catalyzed by Fe-containing Nitric Oxide Reductase (NOR): $2NO + 2e^- + 2H^+ \rightarrow N_2O + H_2O$. So, there should be a mechanism which promotes a smooth transfer of NO from water-soluble NiR to membrane-integrated NOR.

We tried to co-crystalize NOR and NiR, and succeeded in structural determination of NOR/NiR complex[1, 2]. On the basis of this crystal structure, we have proposed that NiR dimer attaches NOR monomer in the cellular system, as shown in Figure 1. In the interface of NOR-NiR interaction, in addition to van der Waal contact, electrostatic interaction of Arg71 (NiR) - Glu119 (NOR) was found. Mutation of negatively charged Glu119 to positively charged Arg retarded growth of the bacterium, suggesting that the interaction between NOR and NiR is responsible for the bacterial survival. Molecular dynamic simulation, which was carried out by the RIKEN Sugita's group,

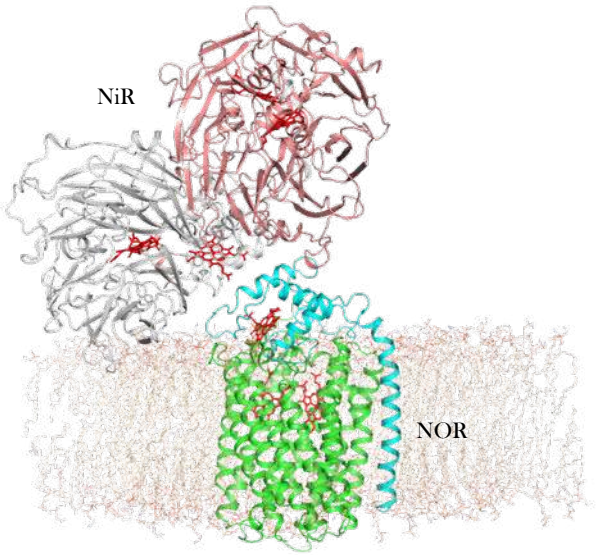

Figure 1. Structure of NiR-NOR Complex

showed that hydrophobic NO molecule produced by NiR could rapidly move from aqua-phase to cellular membrane, and then migrate into the active site of NOR through the hydrophobic channel. These observations suggested that, upon the complex formation, the water-soluble NiR can be located in close proximity of both cellular membrane and NOR for rapid decomposition (detoxification) of NO without diffusing it into the cell. This was a first report to discuss the NO dynamics in cellular system in structural terms of the related enzymes.

2. Oxygen Sensing FixL/FixJ System

Oxygen (O_2) is an important element for life, e.g., for aerobic respiration, it is a resource of our living energy, while, for anaerobic living microorganisms, it is highly toxic. Nitrogenase in root nodule bacteria can catalyze the nitrogen fixation reaction ($N_2 + 6e^- + 6H^+ \rightarrow 2NH_3$), which is also a part of the global nitrogen cycle. Since nitrogenase is labile under aerobic condition, the rood nodule bacteria regulate expression of this enzyme in genetic level in response to the O_2 concentration in soil. So the bacteria have the O2 sensing system, so-called FixL/FixJ system. This system consists of two proteins FixL (histidine kinase) and FixJ (response regulator). The O_2 binding to the heme iron (Fe) in the sensor domain of FixL acts as a triger to induce the conformational change of the histidine kinase domain, resulting in phosphor-transfer reaction from ATP to FixJ. Thus, elucidation of interactions of domain-domain in FixL and of FixL-FixJ is quite important to understand the intra-molecular and inter-molecular signal transduction in the O_2 sensing mechanism. For this purpose, we characterized the FixL-FixJ complex structure in solution by the small angle scattering techniques[3]. Since the crystallographic analysis of such multi-domain proteins was quite difficult, our result provided a first description of the overall structure, but not in an atomic level, of the O_2 sensing system (Figure 2).

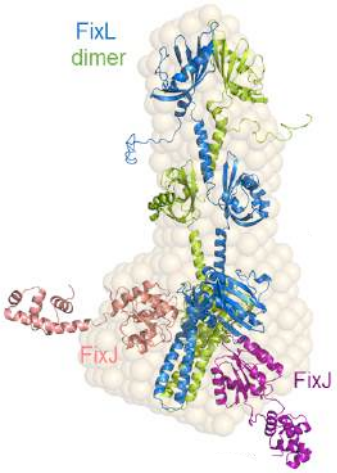

Figure 2. Structure of FixL-FixJ Complex

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意義と波及効果：タンパク質に代表される生体高分子と他の分子（他のタンパク質、核酸、基質など）やイオンなどとの**相互作用**は、細胞機能にとって極めて重要かつ本質的なプロセスであり、その**相互作用**の実態を明らかにすることは細胞機能を理解する、すなわち生命を理解するためには欠かせない研究である。本研究では、地球上での窒素サイクルにとって重要な「脱窒」（微生物の嫌気呼吸の一つ）と、微生物の生存に必須な「酸素濃度感知」をターゲットにし、これらの生理機能において重要な働きをしているタンパク質における相互作用の実態を構造生物学的な手法で明らかにした。生命現象における相互作用の意義を、分子レベルで解明し、原子・電子レベルで議論した重要な研究成果である。

[Category 1]

Directed self-assembly of nanoparticles using DNA terminal-specific interaction

（DNA 末端間相互作用で配向制御したナノ粒子の自己組織化）

Tohru Takarada[1], Li Yu[1], Guoqing Wang[2], Yoshitsugu Akiyama[3], Naoki Kanayama[4], and Mizuo Maeda[1]

[1] Bioengineering Laboratory, RIKEN, [2] College of Food Science and Engineering, Ocean University of China, [3] Faculty of Industrial Science and Technology, Tokyo University of Science, [4] Graduate School of Medicine, Science and Technology, Shinshu University

In nanobiotechnology, special interest has been converging on gold nanoparticles densely functionalized with single-stranded DNA (ssDNA–AuNPs). This is because the particles show beneficial traits that arise from a combination of base complementarity of DNA and physical/chemical properties of AuNP. In 2003, our group identified their extraordinary colloidal behaviors (Fig. 1).[1,2] The ssDNA–AuNPs remain stably dispersed even in an aqueous medium of high ionic strength, due to an interparticle electrostatic and steric repulsion. By contrast, when the complementary ssDNAs are added to form DNA duplexes on the AuNP surface, the resultant double-stranded (ds) DNA–AuNPs are spontaneously and rapidly aggregated under the same conditions. Interestingly, the dsDNA–AuNPs continue to stably disperse when a terminal mismatch exists on the periphery of the dsDNA layer surrounding the AuNP core. An investigation using colloidal probe atomic force microscopy suggested that the interparticle attractive forces were dominated by π–π stacking interaction between the base pairs at the solution-facing termini.[3] In this research project, we have been trying to apply the unique colloidal properties to directed self-assembly of DNA–AuNPs towards development of new methods to construct functional nanomaterials. Below we summarize three achievements.

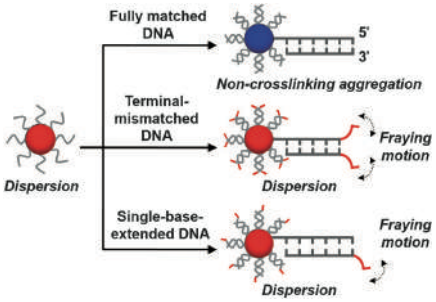

Figure 1. Schematics of the colloidal behaviors of DNA–AuNP.

Directed Assembly of Anisotropic Nanoparticles. Initially, we focused on structurally anisotropic gold core, instead of isotropic spheres that have consecutively been used. Gold nanorods (AuNRs) region-selectively modified with different ssDNA spontaneously formed side-by-side and end-to-end assemblies in a non-crosslinking manner (Fig. 2).[4] When the complementary ssDNA was hybridized to the surface-grafted ssDNA, stacking interaction between the blunt ends took place in the designated regions. Such AuNRs assembled into highly ordered structures, assisted by capillary forces emerging during evaporation on the substrate surface. Furthermore, insertion of a mercury(II)-mediated thymine–thymine base pair into the periphery of the DNA layer allowed selective formation of the side-by-side or end-to-end assemblies from the strictly identical AuNRs with or without mercury(II). Similar directed assembly was also achieved using gold nanoplates region-selectively modified with different ssDNA.[5]

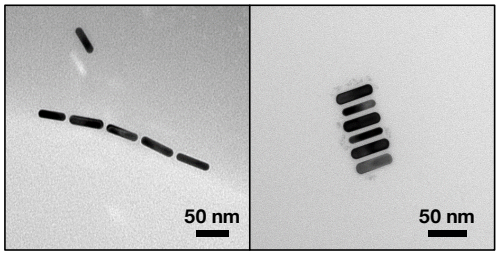

Figure 2. TEM images of end-to-end (left) and side-by-side (right) assemblies of DNA–AuNRs.

Directed Assembly of Nanoparticle Oligomers. Linear AuNP trimers were prepared by aligning both the fully matched and terminal-mismatched dsDNA–AuNPs on a DNA template in a defined order. The trimer underwent directed assembly, as revealed by electron microscopy (Fig. 3).[6] The identity of the central particle controlled the structural anisotropy. The trimers containing the terminal-mismatched or fully matched dsDNA–AuNP at the center selectively assembled in an end-to-end or side-by-side manner, respectively. Further, similar trimers having a central terminal-mismatched particle larger than the peripheral fully matched one formed assemblies that had small particles between the large particles. By contrast, the trimers with a central fully matched particle larger than the peripheral terminal-mismatched one formed an assembled structure in which the large particles were surrounded by the small particles. The anisotropy was programmable by the rule that an interparticle attractive force emerges only between the fully matched particles.

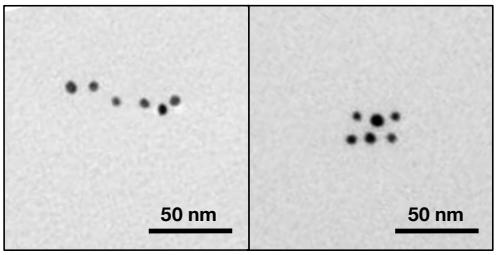

Figure 3. TEM images of end-to-end (left) and side-by-side (right) assemblies of DNA–AuNP trimers.

Folding of Nanoparticle Chains. Longer chains of fully matched dsDNA–AuNPs (>100) underwent shrinkage and folding on the substrate surface (Fig. 4).[7] Specifically, ssDNA–AuNPs were hybridized to a long repetitive ssDNA synthesized with rolling circle amplification to produce the precursory chains. TEM analysis revealed that the chains of fully matched dsDNA–AuNPs were folded to afford the two-dimensional AuNP arrays. In particular, the chains of dsDNA–AuNPs with short interparticle spacing formed the AuNP arrays with anisotropic interparticle spacing. This approach could be useful for readily aligning AuNPs on the substrate surface.

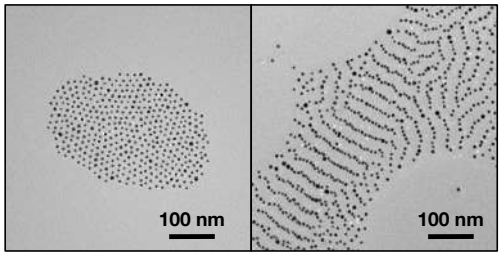

Figure 4. TEM images of two-dimensional arrays of DNA–AuNPs with isotropic (left) and anisotropic structures (right).

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意義と波及効果：構造と物性が等方的なメゾスコピック・スケールの金属微粒子からなる集合体に、構造異方性を誘導する新しい方法論を提案した。これは、分散安定性の異なるナノ粒子を DNA の相補性を利用して順序を厳密に規定して配置し、DNA 末端間**相互作用**を空間的にデザインすることで達成された。特にナノ粒子３量体の配向制御は、両親媒性低分子化合物（界面活性剤）や両親媒性ブロック・グラフト共重合体などの自己組織化との類似性が指摘できる。集合体を構成するナノ粒子の数と順列を拡張すれば、これらの物質と同じくロッド型やベシクル型などの様々なナノ粒子集合体を構築できる可能性があり、次世代のデバイス作製に有用と考えられる。

[Category 2,1]

Measurement of the proton Zemach radius with laser excitation spectroscopy of muonic hydrogen

（ミュオン水素原子のレーザー分光による陽子 Zemach 半径の測定）

Katsuhiko Ishida[1], Msasahiko Iwasaki[1], Sohtaro Kanda[1], Yue Ma[1], Shu Aikawa[1], Hideki Ueno[2], Aiko Takamine[2], Satoshi Wada[3], Norihito Saito[3], Masaki Yumoto[3], Katsumi Midorikawa[3], Shinji Okada[4], Masaharu Sato[5], Yu Oishi[5], and Yasuyuki Matsuda[6]

[1]Meson Science Laboratory, RIKEN, [2] Nuclear Spectroscopy Laboratory, RIKEN, [3]RIKEN Center for Advanced Photonics, RIKEN, [4]Atomic, Molecular, and Optical Physics Laboratory, RIKEN, [5]High Energy Accelerator Research Organization (KEK), [6]Graduate School of Art and Science, The University of Tokyo

The proton and the hydrogen are the fundamental constituents of the matter composing the universe. They are also the playground of high precision measurements and contributed to the formation of basic ideas of the fundamental physics. On the other hand, our understanding of the proton's inner structure is far from satisfactory yet. Recently, a surprise came out when the high-precision result of the proton *charge radius* was published[1] in 2010. It showed a radius with more than 5σ deviations smaller than the average of the previous measurements. This discrepancy, "proton radius puzzle", still remains unsolved in spite of many works both experimentally and theoretically.

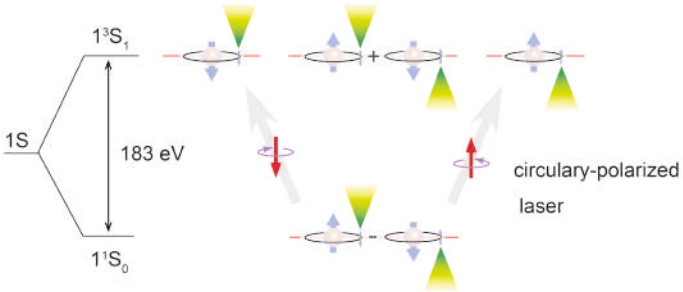

Fig. 1 Scheme of the HFS measurement. By irradiating a circularly polarized laser of the right wavelength, a selected state of the triplet is fed, resulting in the muon spin polarization followed by asymmetric emission of an electron when the muon decays.

In order to shed light on the puzzle, we propose to determine the proton *Zemach radius*, which is defined as a convolution of the charge distribution and the magnetic moment distribution. The proton Zemach radius can be derived from the hyperfine splitting (HFS) of the muonic hydrogen atom. There has been only one measurement using muons so far, which is indirect as a difference between two transitions in the excited states and had 3% error. We plan a new measurement to better than 1% precision by directly exciting the transition between 1s hyperfine states of the muonic hydrogen[2]. This will clarify whether the muon anomaly exists in Zemach radius also or not.

There has been no measurements of the hyperfine splitting of the muonic hydrogen in the ground state so far because the transition is slow as it is E1 forbidden and also there has been no good detection methods. We propose a new method utilizing the muon spin polarization caused by circularly polarized laser (Fig. 1). We are developing the key techniques such as the production of large amount of muonic hydrogen atoms and the high-intensity mid infra-red laser.

We need a 6.8 μm laser with 20 mJ pulse power and frequency broadening of 100 MHz to excite the hyperfine transition. There is no coherent laser available that can directly produce this wave length, so we plan a wave length conversion with optical parametric oscillation (OPO) using ZGP crystal. The scheme under development is shown in Fig. 2. We are testing the Tm, Ho:YAG laser, and confirmed the generation of 2.09

μm laser with pulse width less than 150 ns, which will be used as an input for wavelength conversion and amplification with OPO and OPA[3].

For the formation of muonic hydrogen, we studied the stopping of negative muons in hydrogen gas at the RIKEN-RAL Muon Facility. By choosing the low momentum muons, we confirmed that a good stopping efficiency can be expected even for a density gas with density as low as 0.1% of the liquid hydrogen.

One essential requirement from this method is that the muon spin polarization formed by the laser excitation is held until the polarization is detected by the muon decay. The largest obstacle is the spin depolarization by the inelastic collision with surrounding hydrogen atoms, for which rate there has been only theoretical calculations. In order to measure the rate, we carried out the muon spin rotation measurement first with the deuterium gas in Sep 2018. When polarized negative muons are injected in a deuterium gas, the formed muonic atom is expected to have some residual muon spin polarization. The spin precession of the muonic deuterium was observed under the applied transverse field of 12 mT by the asymmetric decay of the muon decay electrons as in Fig. 3. This was the first clear observation of the precession spectrum at low density as low as 0.1 % of the liquid hydrogen density (LHD). The result is being interpreted with the cascade model in the muonic atom.

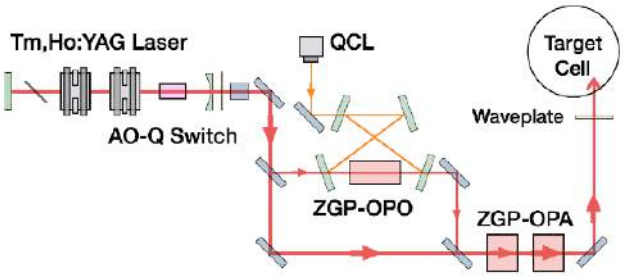

Fig. 2: Schematics of the mid-infrared laser.

After the successful measurement with muonic deuterium, we carried out the measurement with muonic hydrogen in Dec 2019. Muonic hydrogen is expected to have higher collisional de-excitation rate, so we had to decrease the density further down to 0.005% of LHD to hold the polarization, which resulted in smaller muon stopping efficiency. Even though, we obtained a signal which will be attributed to the muon spin precession. The data is under detailed analysis.

Towards the realization of the laser resonant excitation measurement, we are progressing improvement of the laser system with further tuning, doubling of the light source, and the design of the laser cavity in the target cell.

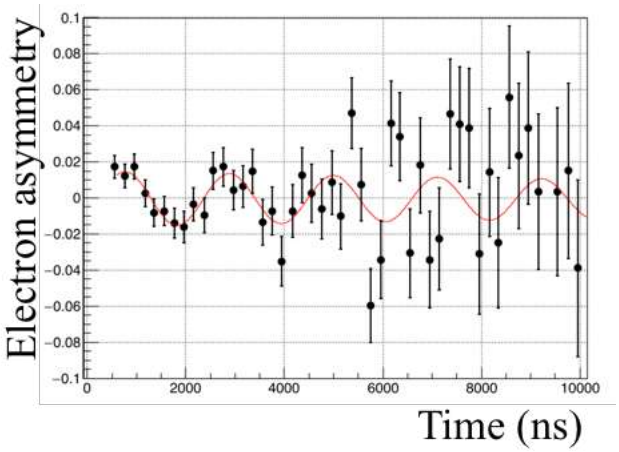

Fig. 3: Muon spin precession spectra of μ^-d

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意義と波及効果：本研究は陽子の大きさという宇宙の主要構成物質に関わる研究である。陽子サイズは量子色力学（QCD）から計算可能な量であり、その正確な値の理解は QCD の検証にもつながる。また陽子半径パズル（プローブによる食い違い）は素粒子レプトンである電子とミュオンの統一性にも挑戦する課題である。一方、実験に用いるレーザー技術は中赤外領域においてこれまでにない高強度・高精度・高安定性を目指すものであり環境モニタリングなどへの応用の可能性も含んでいる。これまでにミュオンビームも含めた実験技術の開発を進めるとともに、ミュオン水素原子自体の研究においても残留偏極度測定という成果を得ている。

[Category 2]

Development of a High-Throughput, Trigger-Less Data Acquisition System for the Excited Charm Baryon Spectroscopy Experiment

（チャームバリオン分光実験のための高効率トリガレスデータ収集システムの開発）

R. Honda[1], Y. Igarashi[2], Y. Ma[3], H. Noumi[4], T. N. Takahashi[5], K. Shirotori[4] and for the J-PARC E50 Collaboration

[1] Graduate School of Science, Tohoku University, [2] Institute of Particle and Nuclear Studies, KEK, [3] Meson Science Laboratory, RIKEN, [4] Research Center for Nuclear Physics, Osaka University, [5] Radiation Laboratory, RIKEN

As a next generation high luminosity hadron and nuclear physics experiment, J-PARC E50 requires measurement of multiple reaction channels simultaneously with enormous amount of data from detectors. Traditional counter experiments with hardware event trigger technique cannot fulfill such requirements. Therefore, we propose to develop a high-throughput trigger-less data acquisition system (DAQ) to face this challenge. The proposed DAQ has the following features: 1) capability to handle MHz order event rate and a data throughput of 10GB/s in average; 2) optimized online filtering and tracking algorithm to select physics event effectively with 99% background suppression; 3) entirely implemented with general purpose computing devices (CPU and GPU).

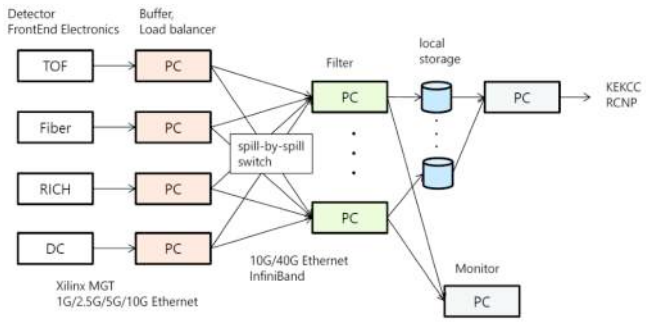

Figure 1: Concept of the streaming DAQ system

The concept of the proposed DAQ is illustrated in Fig.1. There are four stages in the proposed trigger-less

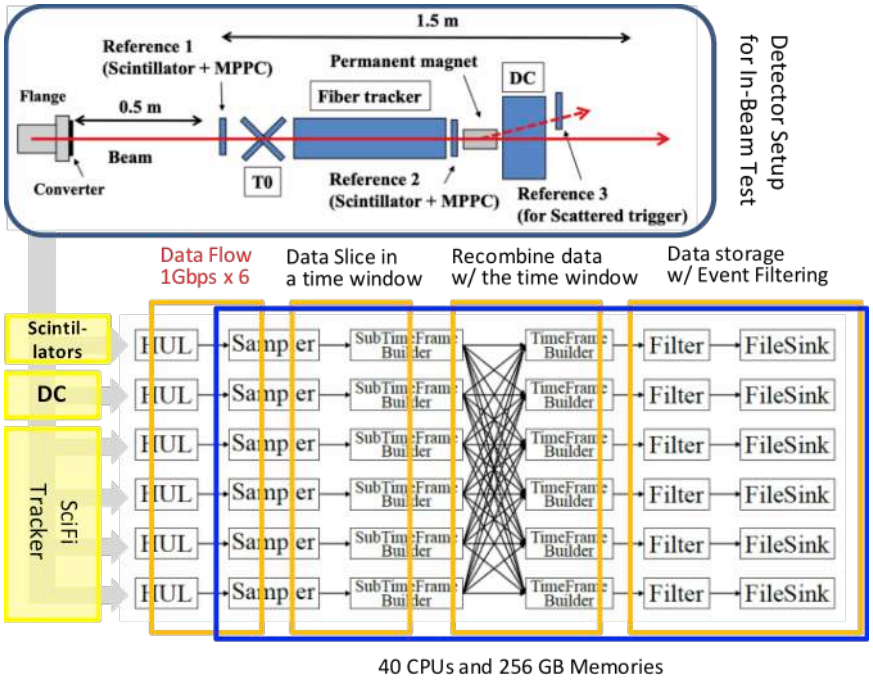

Figure 2: In-Beam Setup and Data Flow in the Streaming DAQ system

DAQ: buffering, packing, tracking and storing. The digitized signals from detectors (TDC and ADC) carrying global time stamp are sent to buffer stations first via fast Ethernet connection. Data from different detectors are merged and packed into event candidates at packer stations. The packed events are then fed into tracker stations as shown in Fig.1, where data filtering and tracking are performed by software. Only charm related physics events passed those filtering and tracking are saved into local storage devices for offline data analysis.

We have developed FPGA based streaming TDC modules with synchronization capability. A prototype DAQ software was prepared based on FairMQ [1]. We have carried out in-beam test for the idea of streaming DAQ in December of 2018, at ELPH of Tohoku University, which clearly demonstrates the feasibility of the proposed setup. The schematic setup used for the in-beam test is shown in Fig.2. In total, 128 channels of scintillation fiber, 14 channels scintillation counter and 30 channels of drift chamber are read by six streaming TDC modules without trigger selection. All six streaming TDC modules (HUL [2]) worked at their highest throughput (1Gpbs) without obvious data loss. This is an important evidence for the transportation capability of TCP/IP technique in near real time condition.

During the in-beam test, we tested two types of online processing algorithm to pack data from different TDC modules together and suppress random hits from detectors. The first method is to employ standard C++ algorithm (inplace_merg()) to merge and sort the TDC data. The online performance was found that one needs ~25GB RAM and ~25 CPU cores to handle 6Gbps data throughput. However, the performance is also strongly dependent on the data segment size: a smaller data segment to be processed the better performance can be expected. There is still some possibility to optimize this method by fine tuning the data segment. Another method we tested is named as fixed time window method. We divide the global TDC data into 1μs wide time window, which is mapped to a fixed address in RAM space. By checking the multiplicity information of each time window, we will be able to suppress the dark counts from hot channels. The performance of this method is given in Fig.3. It is apparent that this method is more economic and allow us to perform further online processing such as hit position finding by using pre-built look-up table. In any case, we have achieved an important goal by demonstrating the data processing capability of modern server machine and established the feasibility of streaming DAQ.

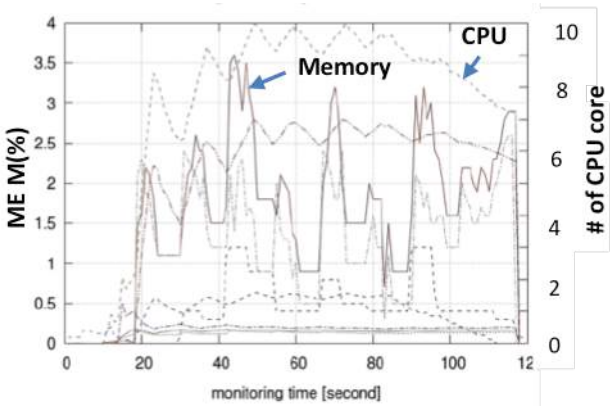

Figure 3: CPU and Memory Consumption among 40 CPUs and 256 GB Memories

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意義と波及効果：従来の素粒子原子核実験におけるデータ収集（DAQ）システムは、特定の事象を選別するトリガー信号によって検出器からのデータをデジタル化し計算機上の記憶装置に記録する方式が一般的である。近年の大規模加速器実験では、検出器の種類や数が膨大、かつ、事象も多岐にわたり、トリガー信号の生成も複雑になる。トリガーを排除した DAQ システムの開発は時代の要請である。トリガーを廃した代償はネットワーク上を流れるデータ量負荷の増大となるが、これを適切な並列計算機群で分散処理を行うことでほぼ100%の効率を達成できる。事象の選別（データを記録するかどうかの判断）はソフトウエア上で行うので汎用性および可搬性に優れる。実験規模に応じた並列処理システムを導入すれば、広く普及が期待できる。

[Category 2]

Deformation of the excitation state in RI far from the beta-decay stability investigated through the measurement of nuclear moments

（核モーメント測定で探るベータ崩壊安定線から遠く離れたRIの励起状態核変形）

Y. Ichikawa,[1] H. Nishibata,[1,4] Y. Tsunoda,[5] A. Takamine,[1] K. Imamura,[1,6] T. Fujita,[1,4] T. Sato,[1,7] S. Momiyama,[8] Y. Shimizu,[2] D. S. Ahn,[2] K. Asahi,[3,7] H. Baba,[2] D. L. Balabanski,[1,9] F. Boulay,[1,10,11] J. -M. Daugas,[1,11] T. Egami,[12] N. Fukuda,[2] C. Funayama,[7] T. Furukawa,[14] G. Georgiev,[14] A. Gladkov,[1,16] N. Inabe,[2] Y. Ishibashi,[1,17] T. Kawaguchi,[12] T. Kawamura,[4] Y. Kobayashi,[1,18] S. Kojima,[7] A. Kusoglu,[9,15,19] I. Mukul,[110] M. Niikura,[8] T. Nishizaka,[12] A. Odahara,[4] Y. Ohtomo,[1,7] T. Otsuka,[1,5,8,20] D. Ralet,[15] G. S. Simpson,[21] T. Sumikama,[2] H. Suzuki,[2] H. Takeda,[2] L. C. Tao,[1,22] Y. Togano,[2,7] D. Tominaga,[12] H. Ueno,[1] H. Yamazaki,[1] and X. F. Yang[20]

Nuclear Spectroscopy Laboratory, RIKEN,[1] BigRIPS Team, RIKEN Nishina Center,[2] RI Physics Laboratory, RIKEN Nishina Center,[3] Department of Physics, Osaka University,[4] Center for Nuclear Study, University of Tokyo,[5] Department of Physics, Meiji University,[6] Department of Physics, Tokyo Institute of Technology,[7] Department of Physics, University of Tokyo,[8] ELI-NP, IFIN-HH,[9] GANIL, CEA/DSM-CNRS/IN2P4,[10] CEA, DAM, DIF,[11] Department of Advanced Sciences, Hosei University,[12] Department of Physics, TokyoMetropolitan University,[14] CSNSM, CNRS/IN2P4, Universitè Pris-Sud,[15] Department of Physics, Kyungpook National University,[16] Department of Physics, University of Tsukuba,[17] Department of Informatics and Engineering, University of Electro-Communications,[18] Department of Physics, Istanbul University,[19] Department of Particle Physics, Weizmann Institute,[19] Intsituut voor Kern-en Srralingsfysica, K. U. Leuven,[20] LPSC, Universitè Grenoble Alpes, CNRS/IN2P4,[21] School of Physics, Peking University[22]

Exotic nuclei are characterized by a number of excess neutrons (or protons) relative to stable nuclei. Their shell structure, which represents single-particle motion in a nucleus, may vary owing to nuclear force and excess neutrons, in a phenomenon called shell evolution. This effect could be counterbalanced by collective modes causing deformations of the nuclear surface. We studied the interplay between shell evolution and shape deformation by focusing on the electromagnetic (EM) nuclear moment of an excited (isomeric) state of the neutron-rich nucleus ^{75}Cu,[1] where low-lying states of the Cu isotopes exhibit an intriguing behavior involving the shell evolution.[2–4]

Experimentally, however, it is not easy to perform the nuclear EM moment measurements for such extremely neutron-rich nuclei using conventional experimental methods. In order to determine nuclear EM moment from the anisotropy of the γ rays emitted, we have to produce the nuclear spin alignment. In the case of extremely neutron-rich nuclei such as ^{75}Cu, a new method to collect the RIs efficiently while producing the large nuclear spin alignment is indispensable because of the very low production yields. Recently, the "dispersion-matching two-step projectile-fragmentation (PF) method" has been developed as a new spin manipulation technique for RI beams.[5] This method obtains an RI beam with a high production yield while producing universally high spin alignment for a large variety of RIs. A proof-of-principle experiment was performed at the RIBF facility. The application of this method has enabled the measurement for ^{75}Cu.

The magnetic moment measurement was carried out at the BigRIPS at RIBF. Spin alignment as large as 30% was achieved in the isomeric state of ^{75}Cu by a scheme of two-step projectile fragmentation with a technique of momentum-dispersion matching,[5] incorporating an angular-momentum selecting proton removal from ^{76}Zn. The magnetic moment was determined using the time-differential perturbed angular distribution

(TDPAD) method. Owing to the high spin alignment realized by the refined two-step scheme, the observed oscillation for the 66.2-keV γ rays in the TDPAD spectrum had a significance greater than 5σ. The magnetic moment of the 66.2-keV isomer with spin parity $I^{\pi} = 3/2^{-}$ was determined to be $\mu = 1.40(6)\ \mu_N$.

The magnetic moment, thus obtained, demonstrated a considerable deviation from the Schmidt value, $\mu = 3.05\ \mu_N$, for the $p_{3/2}$ orbital. Figure 1 shows the systematics of magnetic moments of the $3/2^{-}$ and $5/2^{-}$ states, where deviation from the Schmidt values appears to be maximal at ^{75}Cu. The analysis of the magnetic moment with the help of Monte Carlo shell model (MCSM) calculations[7] reveals that the trend of the deviation corresponds to the effect of core excitation and the low-lying states in ^{75}Cu are, to a large extent, of a single-particle nature on top of a correlated ^{74}Ni core, elucidating the crucial role of the shell evolution even in the presence of collective mode.[6]

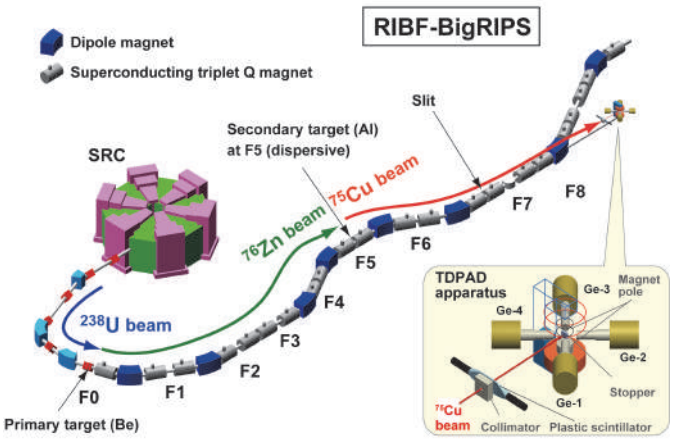

Figure 1 Arrangement of the BigRIPS RI separator for the present spin-aligned ^{75}Cu beam under the scheme of dispersion-matching two-step nuclear reaction.

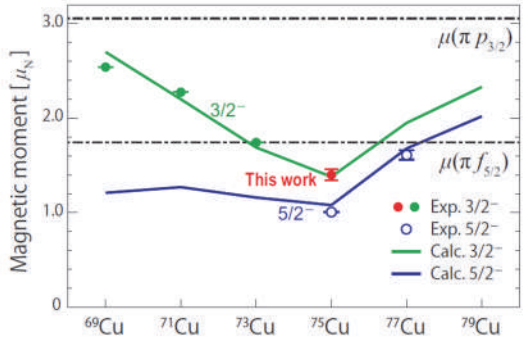

Figure 2 Systematics of magnetic moments for odd-*A* Cu isotopes. Filled and open circles represent experimental data for $3/2^{-}$ and $5/2^{-}$ states, respectively. Filled red circle represents the result obtained in this work. Solid green and blue lines represent MCSM calculations for $3/2^{-}$ and $5/2^{-}$ states, respectively, with $20 \leq (N, Z) \leq 56$ model space. $\mu(\pi p_{3/2})$ and $\mu(\pi f_{5/2})$ denote the proton Schmidt values for $p_{3/2}$ and $f_{5/2}$, respectively.

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意義と波及効果：核電磁モーメントは核内部の波動関数（核配位）を最も先鋭に反映する観測量の一つで、核構造研究では異常性特定の決定的手段として用いられることも多い。しかし測定は困難な部類に入り、特に遠中性子委過剰核では観測例は限定的である。本研究はこれを可能とした技術的ブレイクスルーの最初の本格的適用として ^{75}Cu という遠中性子過剰核の核磁気モーメント測定に成功したものである。得られた結果は京コンピュータを用いた大規模殻模型計算を用いて分析され、実験と理論を合わせて 75Cu 核の性質解明に大きく貢献している。当該手法の本格的利用に成功したことにより、今後励起状態（アイソマー準位）の核電磁モーメント測定を通じた中性子過剰核の構造研究が広く展開されると期待される。

[Category 2]

Radiative cooling dynamics of excited molecular ions stored in RICE

（RICE 中に蓄積された励起分子イオンの放射冷却ダイナミクス）

T. Azuma[1], N. Kimura[1], ∗ S. Kuma[1], K. C. Chartkunchand[1], P. M. Mishra[1], T. Yamaguchi[2] and Y. Nakano[3]

[1]AMO Physics Laboratory, RIKEN, [2]Department of Physics, Saitama University

[3]Department of Physics, Rikkyo University

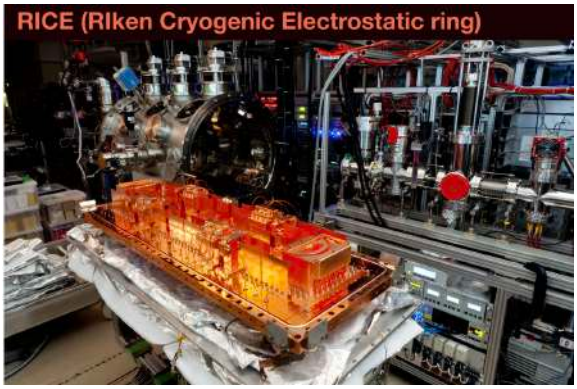

Figure 1 Photo of electrodes of RIKEN Cryogenic Electrostatic Ion Storage ring (RICE)

The RIKEN Cryogenic Electrostatic Ion Storage ring (RICE) has been operated at cryogenic temperatures down to 4.2 K [1], which enables the storage of the atomic and molecular ions for the long period of the order of 1000 s or longer. RICE opened a new opportunity to study slow excitation and de-excitation dynamics of molecular ions through observation of the time evolution of the populations at the specific vibrational and rotational levels, which is one of the cutting edge topics in the present atomic and molecular physics.

We studied the radiative cooling process of a triatomic molecular stored in RICE, which possesses a new challenge on understanding the quantum systems at the discrete level region with multiple degree of freedom. In general, rotational and vibrational RC processes of triatomic molecules are slow, which has never been explored before, due to small permanent dipole moments. Additionally, the increased number of degrees of freedom: multiple vibrational and rotational modes and their mutual interactions make the dynamics much more complicated. We employed N_2O^+ possessing three vibrational modes (v_1 v_2 v_3) as the target of our study. This molecule is known to produce neutral fragments by photodissociation, and the distribution of rotational and vibrational states in the $X^2\Pi$

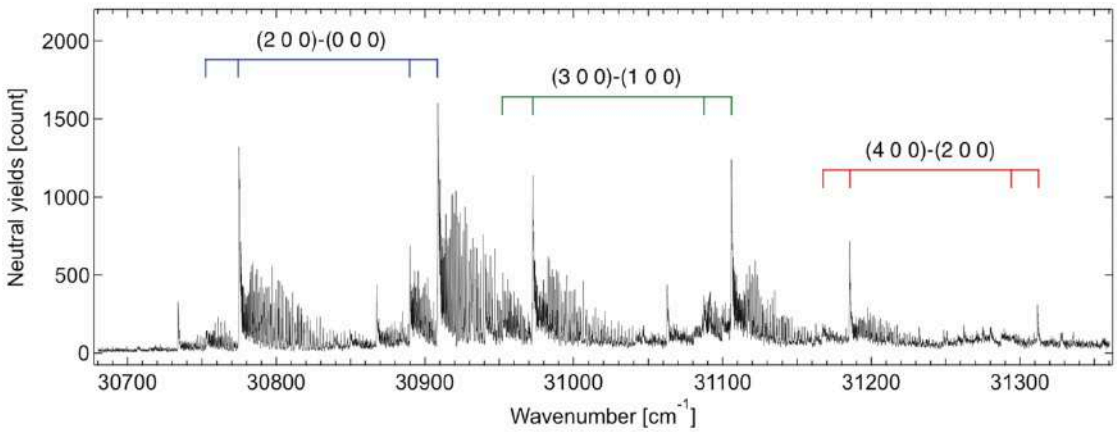

Figure 2 $A^2\Sigma^+$-$X^2\Pi$ photodissociation spectrum of N_2O^+ measured at a storage time of 9 ms. The wavelength region corresponds to the vibrational excitation of Δv_1= v'-v''=2 sequence, with the main features attributed to the rotational band heads of the (v'00)-(v''00).

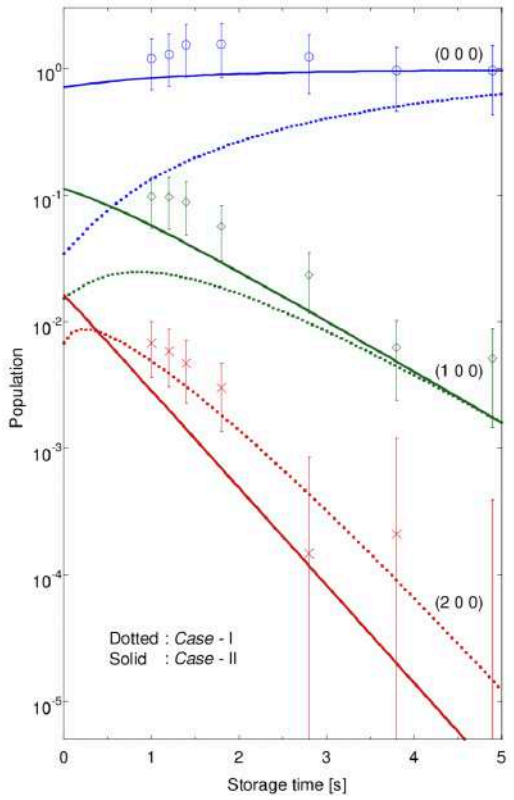

Figure 3 Observed and simulated population evolutions for vibrational states as a function of ion storage time. The solid and dotted lines represent simulation results under initial distributions in thermal equilibrium and non-equilibrium, respectively.

electric ground state can be evaluated by predissociation processes via the $A^2\Sigma^+$ excited bound state using photons in the readily accessible near-ultraviolet (UV) wavelength range. The temporal evolution of their population can be conveniently monitored by changing the timing of the laser irradiation after the ion storage.

Figure 2 is a typical example of the spectrum obtained as a function of the laser wavelength. We thus succeeded in obtaining a high-resolution rovibrational spectrum showing the detailed rotational level population, the quality of which is far better than previously measured by the conventional technique. Furthermore, we focused on three $\Delta = +2$ transitions for the symmetric stretching vibration of ν_1. We traced the evolution of the relative intensity of these yields by changing the timing of the laser irradiation. As shown in Fig.3, we found the significant radiative cooling behavior for the vibrationally excited states of (1 0 0) and (2 0 0) over a period of several seconds, while noticeable increase of the population of the ground state (0 0 0) was not observed. Supported by theoretical simulations of the population evolution, we concluded that the initial ion production by electron impact via Franck-Condon-type transitions in the ion source explains our observation rather than a naive Boltzmann-type distribution. We pointed out that we can reach the conclusion, because the population distribution in each mode reflects its specific character in such multi-mode system. This discussion is in contrast to diatomic molecules that have been intensively studied in the past. Thus, our study will open a new insight for understanding the radiative cooling dynamics of polyatomic molecules having rich internal degrees of freedom.

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[3] A. Hirota, R. Igosawa, N. Kimura, S. Kuma, K. C. Chartkunchand, P. M. Mishra, M. Lindley, T. Yamaguchi, Y. Nakano and T. Azuma, Phys. Rev. A. *to be submitted.*

意義と波及効果：最近のイオン蓄積リングやイオントラップの技術的進展により、真空中に孤立した１分子を長時間にわたって観測することが可能になってきた。そこでは今まで不可能であった、従来の統計力学による集団の平衡状態における振る舞いの記述を超えた、量子準位ごとの時間発展を追跡することができる。我々は研究室で独自に開発した極低温イオン貯蔵リングを利用して、真空中に孤立した分子イオンの長い時間領域における励起および脱励起ダイナミクスを探求してきた。今まで研究対象とされてきた２原子分子ではなく、直線３原子分子イオン(N_2O^+)を対象として初めて選び、準位ごとの振動冷却過程の秒オーダーのダイナミクスを明瞭に捉えることに成功した。この手法は、さまざまな分子に適応することが可能である普遍的なアプローチであり、熱浴が 4K である孤立系のダイナミクスを量子力学と統計力学両者を駆使して研究する新しい手法を提供すると期待される。

[Category 2,4]

Excitation of a single molecule by localized surface plasmon

（局所表面プラズモンによる単分子励起）

Emiko Kazuma[1], Jaehoon Jung[2], Hiromu Ueba[3], Michael Trenary[4], and Yousoo Kim[1]

[1]Surface and Interface Science Laboratory, RIKEN, [2] Department of Chemistry, University of Ulsan,
[3] Graduate School of Science and Engineering, University of Toyama,
[4]Department of Chemistry, University of Illinois at Chicago

Plasmon-induced chemical reactions on metal nanostructures have been attracting attention because the plasmon can promote highly efficient conversion from solar energy to chemical energy. However, the reaction mechanism is still controversial mainly because the direct observation of the chemical reactions in the plasmonic field is difficult due to the strong localization of the plasmon near the metal surface. Figure 1 illustrates the decay process of the plasmon and the excitation mechanisms of the molecules.[1] During the excitation and decay processes of the plasmon, the strong electric field (Fig. 1a), electron-hole pairs (Fig. 1b), and heat (Fig. 1c) can be used as excitation sources of the molecules. Plasmon-induced chemical reactions have been explained mainly by an indirect hot-electron transfer mechanism (Fig. 1e).[2,3]. The hot electrons are transferred to form a transient negative ion (TNI) state of the adsorbed molecule. In this study, we propose a direct intramolecular excitation mechanism (Fig. 1d(i)), on the basis of direct observation of a plasmon-induced chemical reaction at the single-molecule level with a scanning tunneling microscope (STM).[4] Dimethyl disulfide, $(CH_3S)_2$, was selected as a target molecule. Our previous work revealed that visible-light-induced photodissociation of the S−S bond in $(CH_3S)_2$ molecules adsorbed on Ag(111) and Cu(111) surfaces occurs through direct electronic excitation from highest occupied molecular orbital (HOMO)- to lowest unoccupied molecular orbital (LUMO)-derived molecular orbitals (the anti-bonding S-S (σ^*_{SS}) orbital).[5]

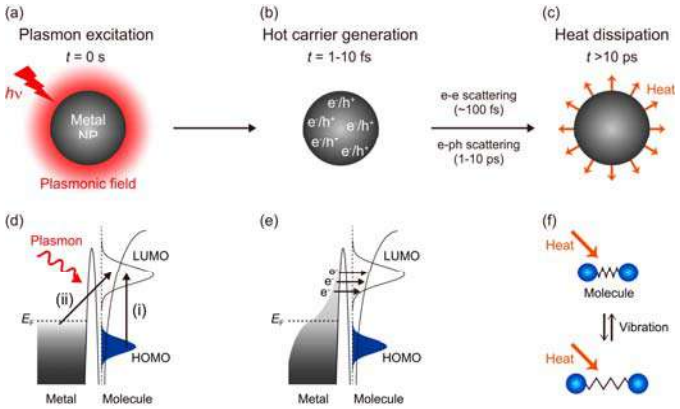

Figure 1 (a) Excitation and (b, c) decay processes of the localized surface plasmon of a metal nanostructure. (d–f) Excitation mechanisms of molecules adsorbed on the metal surfaces during the excitation and decay processes of the plasmon. (d) (i) Direct intramolecular excitation mechanism and (ii) charge transfer mechanism. (e) Indirect hot-electron transfer mechanism. (f) Local heating mechanism. (Ref. 1)

An Ag tip with a curvature radius of ~60 nm was positioned over the metal surface to excite the plasmon optically at the STM junction (Fig. 2a). The S-S bond in $(CH_3S)_2$ was dissociated by the plasmon

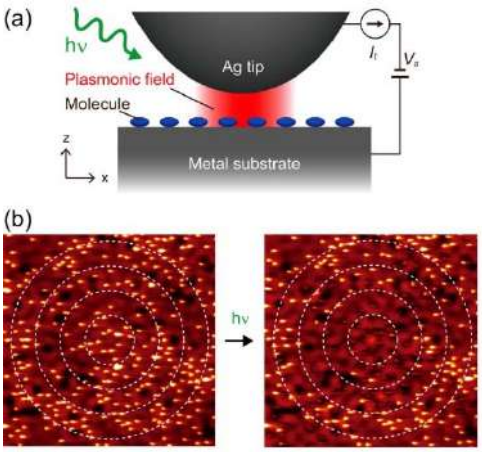

Figure 2 (a) Schematic illustration of the experiment. (b) Topographic STM images of (CH3S)2 molecules on Ag(111) before and after irradiation with p-polarized light at 532 nm. The tip was positioned at the center of concentric rings during light irradiation. (Ref. 4)

preferentially under the tip, which was revealed by the spatial distribution of isolated $(CH_3S)_2$ molecules before and after the excitation of the plasmon (Fig. 2b). From a comparison of the simulated electric field intensity, the plasmon-induced dissociation has a strong correlation with the electric field intensity of the plasmon. The wavelength (λ) dependence of the dissociation yield (*Y*) was also examined, which indicates the plasmon efficiently induces and enhances the dissociation reaction through the same reaction pathway as photodissociation ($n_S \rightarrow \sigma^*_{SS}$).

Real-time observation with the STM in plasmon-induced chemical reactions of single molecules provides insights into the elementary reaction pathways. Tunneling current (I_t) is highly sensitive to the change in the gap distance, and thus dissociation of a single $(CH_3S)_2$ molecule can be detected from a change in I_t when the STM tip is positioned over the molecule under light irradiation (Fig. 3). The reaction pathway initiated from the TNI states formed by electron transfer from the metal to the molecule via an inelastic electron tunneling process should be the same regardless of the excitation source: hot electrons or tunneling electrons. Rotation and dissociation of $(CH_3S)_2$ on Ag(111) were induced through vibrational excitation with inelastically-tunneled electrons at higher energy than ~0.28 eV and ~0.36 eV, respectively. Moreover, dissociation induced with tunneling electrons is accompanied by rotation, which results in small changes of I_t followed by its sudden drop even at 2.3 eV, which is almost equal to the light energy at 532 nm. Therefore, we concluded that the energy of TNI states is dissipated to the vibrationally-excited states resulting in both rotation and dissociation of $(CH_3S)_2$, and rotation is a precursor for dissociation. On the other hand, the plasmon-induced dissociation proceeds through vibrational excitation, current changes due to rotation should appear before the dissociation. However, changes in I_t before the sudden drop were not observed (Fig. 3). This excludes the indirect hot-electron transfer mechanism for the plasmon-induced dissociation of $(CH_3S)_2$.

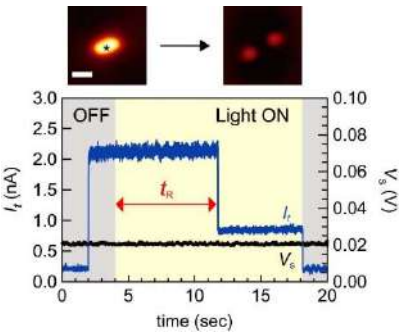

Figure 3 Current trace for detecting the dissociation event of the target molecule (STM images) on Ag(111) induced by the plasmon excited with light at 532 nm. (Ref. 4)

In conclusion, the plasmon-induced dissociation of the S-S bond in a single $(CH_3S)_2$ molecule on Ag(111) and Cu(111) surfaces occurs by the direct intramolecular excitation to the LUMO state of the anti-bonding S-S (σ^*_{SS}) orbital through decay of the optically-excited LSP in the nanogap between the Ag tip and the metal surface. The present results underline that the plasmon-induced chemical reactions of the molecule with the electronic states less hybridized with metals are explained by the direct intramolecular excitation mechanism, but not by the indirect hot-electron transfer mechanism.

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意義と波及効果：本成果は、金属のナノ構造に可視光を照射することで生成するプラズモンによって、分子が**励起**され、高効率の化学反応が誘起されることを示している。今後、分子と金属の界面における相互作用を制御することで、反応に必要な光エネルギーの調節や反応機構の制御ができることから、新しい光触媒の開発につながると期待できる。

[Category 2]

Tracking chemical bond formation with electronic excitation of metal complex assemblies by time-domain Raman spectroscopy

（時間領域ラマン分光を用いた金属錯体会合体の電子励起に伴う化学結合生成の追跡）

Hikaru Kuramochi[1,2,3], Satoshi Takeuchi[i1,2], Munetaka Iwamura[4], Koichi Nozaki[4], and Tahei Tahara[1,2]

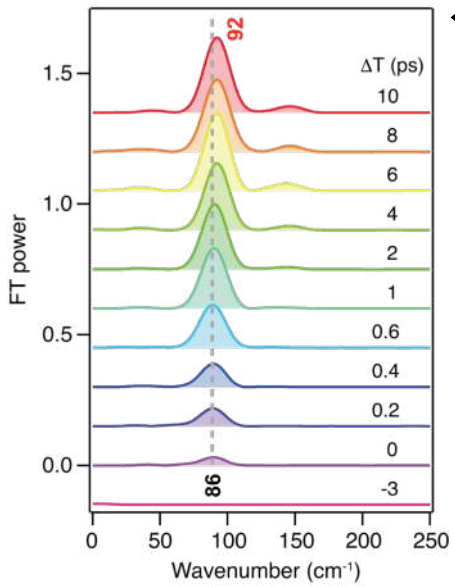
[1] Molecular Spectroscopy Laboratory, RIKEN, [2] Ultrafast Spectroscopy Research Team, RIKEN Center for Advanced Photonics (RAP), [3] PRESTO, Japan Science and Technology Agency, [4] Graduate School of Science and Engineering, University of Toyama

Formation and dissociation of chemical bonds are the heart of chemistry, and elucidation of such a bond rearrangement process is one of the dreams in chemical science. In order to achieve this, we have developed a highly sensitive time-resolved "time-domain" Raman technique, called time-resolved impulsive stimulated Raman spectroscopy (TR-ISRS).[1] TR-ISRS allows us to track structural changes of the photoreaction intermediates with femtosecond time-resolution, and it has been successfully utilized for visualizing ultrafast structural dynamics in the photoreactions of cis-stilbene [2], green fluorescent protein,[3], and photoactive yellow protein.[4] These studies successfully revealed ultrafast structural changes leading to the product state of unimolecular reactions. However, the dynamics of bimolecular reactions with chemical bond formation has been seldom studied not only by the time-domain Raman technique but also by any means.

Oligomers of dicyanoaurate (I) complex ($Au(CN)_2^-$) offer a unique opportunity to investigate the chemical bond formation process. In aqueous solution, the [$Au(CN)_2^-$] complex forms weakly-bonded oligomers $[Au(CN)_2^-]_n$ due to the aurophilic interaction, i.e., an attractive interaction that operates between closed-shell d^{10} Au(I) atoms. Because the aurophilic interaction is as weak as hydrogen bonds (~0.1 eV), the [$Au(CN)_2^-$] complexes are only loosely associated in the electronic ground state. However, the photoexcitation that excites one electron from the anti-bonding σ^* (dz^2 - dz^2) orbital (HOMO) to the bonding σ (p_z - p_z) orbital (LUMO) induces tight Au-Au covalent bond formation (~1 eV) in the excited state, and hence we are able to exmaine the bond formation process with time-resolved spectroscopy. Previously, we studied this system using femtosecond time-resolved spectroscopy, focusing on the observation of coherent nuclear wavepacket motion induced by chemical bond formation. In particular, we studied excited-state dynamics of the [$Au(CN)_2^-$] trimer in aqueous solution using broadband transient absorption spectroscopy in detail.[5] We observed substantial increase of the excited-state absorption signal of the trimer triplet state with the ~2-ps time constant, which we attributed to the bent-to-linear structural change upon the tight Au-Au bond formation. Nevetheless, because the time-resolved absorption spectroscopy is not very sensitive to the molecular structure, the structural details of this ultrafast bond-formation process have not been clarified directly. In fact, a different scheme was proposed after our work. [6] In this study, we realized real-time observation of the ultrafast dynamics of the [$Au(CN)_2^-$] trimer using TR-ISRS.[7] This ultrafast "time-resolved time-domain" Raman technique allows us to monitor the change in the vibrational structure on the femtosecond timescale by inducing and observing coherent molecular vibrations at arbitrary timings. Furthremore, TR-ISRS is very powerful for accessing low-frequency transient Raman bands down to a few terahertz region.

Fig. 1 shows femtosecond time-resolved Raman spectra obtained for the 0.1 M $K[Au(CN)_2]$ aqueous solution, which were obtained as Fourier transform power spectra of the oscillatory signals observed with

time-domain Raman measurments. A distinct transient band is observed at ~90 cm^{-1}, and it grows with the time constant of ~0.4 ps. This band is attributable to the Au-Au strech vibrations of the T_1 trimer, and 0.4 ps corresponds to the $S_1 \leftarrow T_1$ intersystem crossing (ISC) time. Markedly, the frequency of this transient band shifts from 86 cm^{-1} to 92 cm^{-1} with a time constant of 3 ps, which is attributed to bent-to-linear structural change of T_1 trimer based on complementary quantum chemical calclutations. Comparison with the data of more concentrated 0.29 M $K[Au(CN)_2]$ aqueous solution, it turned out that the previous controversy about the assignment of the ultrafast dynamics was caused by the contribution of the excited-state tetramer which coexists in solution. Fig. 2 summarizes the ultrafast dynamics of the photo-induced bond-formation and subsequent structural rearrangements of the $[Au(CN)_2^-]$ trimer.[7] Upon photoexcitation of the weakly associated trimer, the tight Au-Au bond is first formed almost instantaneously. This bond formation causes the rapid shortening of the Au-Au distances, inducing coherent motion along the Au-Au stretch coordinate. Subsequently, the $[Au(CN)_2^-]$ trimer undergoes the ISC with the ~0.4-ps time constant, and then, the bent-to-linear structural change takes place on the T_1 potential energy surface with the ~3-ps time constant. The present study not only settled the controversy but also demonstrates the powerfulness of TR-ISRS in the study of ultrafast structural dynamics of complex molecular systems in general.



← **Figure 1.** Fourier transform power spectra of TR-ISRS signals of the 0.1 M $K[Au(CN)_2^-]$ aqueous solution.

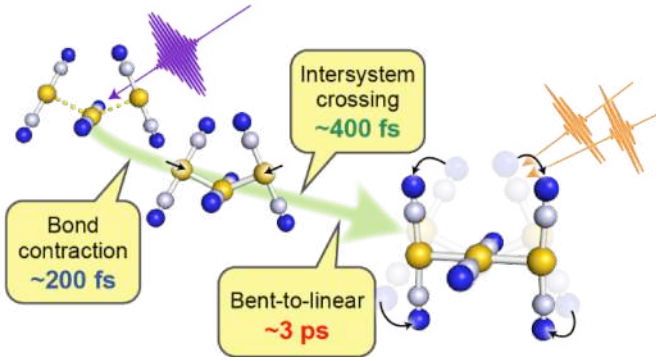


Figure 2. Photo-induced Au-Au bond formation dynamics of the $[Au(CN)_2^-]$ trimer.

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意義と波及効果：

超高速分光による反応ダイナミクス研究は分子科学の主要問題の一つであるが、これまでの研究のほとんどは単分子反応に対するものである。金錯体の会合体では光励起によって金属錯体間に金－金結合が生成するため、分子の間の結合生成とそれに伴う構造変化を実時間で研究することができる。この系に対しては論争があったが、時間領域のラマン分光を用いてダイナミクスを明らかにして論争に決着をつけた。これによって理研で開発された時間分解インパルシブ誘導ラマン分光が複雑分子系の研究に大変強力であることが示された。

[Category 2]

Dynamics of Nitric Oxide in Biological System Examined Using Excitation of Caged NO

（ケージド NO の光励起を活用した、生体内 NO の動態解析）

Yoshitsugu Shiro [1], Kazumasa Muramoto[1], Takashi Nomura[1], Chai Gopalasingam[1], Minoru Kubo[2], Takehiko Tosha[3] and Hiroshi Sugimoto[3]

[1]Cellular Regulation Laboratory, University of Hyogo, [2]Spectroscopy Laboratory, University of Hyogo, [3]RIKEN RSC

Generally, enzymes can catalyze reaction through formation of a short-lived intermediate, i.e., excited state, during its catalytic reaction. To establish the enzymatic mechanism in detail, such intermediates have to be characterized in atomic and electronic level. In our study, we have been trying to establish the reaction mechanism of Nitric Oxide Reductase (NOR) of the denitrification bacteria. This enzyme has an active site consisting of heme *b* and non-heme iron (Fe_B) binuclear center (Figure 1), where two NO molecules are converted into one N_2O molecule ($2NO + 2e^- + 2H^+ \rightarrow N_2O + H_2O$). In this reaction, the N-O bond cleavage and the N-N bond formation are involved through reaction intermediate(s). So far, three types of intermediate, where three types of NO coordination to the binuclear center, have been proposed (Figure 2), but yet not established[1]. So, the reaction mechanism of NOR is still controversial. We have challenged to establish the reaction mechanism by using the time-resolved technique such as pump-probe and cryo-photolysis methods in combinational use of caged NO compound. The caged NO can quantitatively release NO upon the UV flashing, acting as a trigger of the NOR reaction and a NO resource.

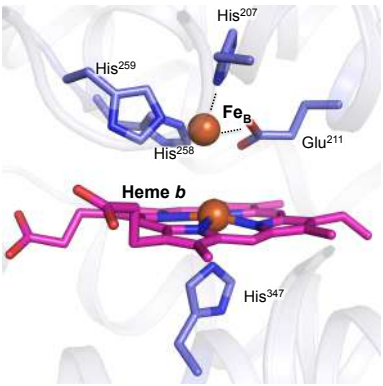


Figure 1 (↑) Active Site Structure of NOR,

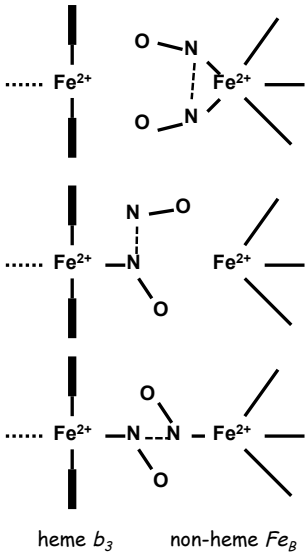


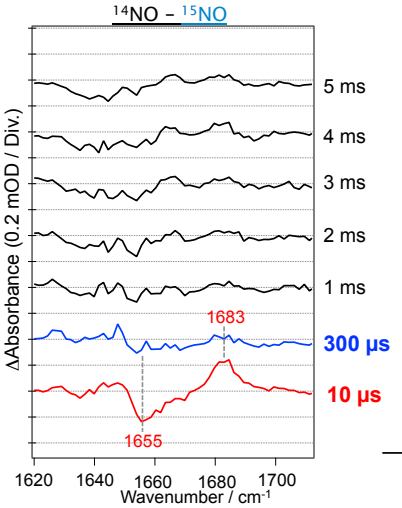
Figure 2 (→) Three Types of Intermediate so far Proposed

1. Kinetic Analysis of the NOR Enzymatic Reaction in Microsecond Time Region[2]

The reaction of NOR in the full reduced (Fe^{2+}) form upon the caged NO photolysis was followed by optical absorption spectoroscopy. The kinetic trace consisted of three phases in the ~μs, ~100μs and ~ms time domains; the reaction rate in the first phase is dependent on the NO concentration, that in the second phase is independent and the third is again dependent on the NO concentration. The observation suggested the presence of two intermediates, I and II, in both of which one NO molecule is present in the active site, but their coordination structure is different. The NO in intermediate II could react another NO molecule in the third phase to give the product N_2O. On the other hand, when we used an inactive mutant of NOR, Glu57Ala, in which the proton transfer was depressed, the third phase was missed, indicating that the protons could be supplied in the third phase to promote the N-N bond formation and the N-O bond cleavage.

2. Time-Resolved IR Spectrum and ESR Spectrum in Cryo-Photolysis of Intermediate I

On the basis of our previous study, it was supposed that the intermediate II has probably in the NO-bound and five-coordinated heme *b* iron in the binuclear center, giving the ESR signal at g = 2 with three super-hyperfine coupling from ^{14}N of NO. Then, for characterization of intermediate I, we applied the pump-probe technique monitored by the IR spectroscopy, to observe the N-O stretching from the NO molecule bound to either heme *b* or non-heme Fe_B. We successfully observed the NO stretching at 1683 cm^{-1} at 10μs after the UV laser photolysis (Figure 3), which was clearly arisen from the intermediate I. On the other hand, we successfully prepared the intermediate I at cryogenic temperature, in which NOR in the fully reduced form was photolyzed in the presence of caged NO and annealing. The resultant ESR spectrum signals at g = 4.1 and 3.9 (Figure 4). Those spectroscopic properties are characteristic of the non-heme iron NO complex reported so far. On the basis of these experimental results, we proposed the molecular mechanism of the NO reduction reaction catalyzed by NOR, as follows.



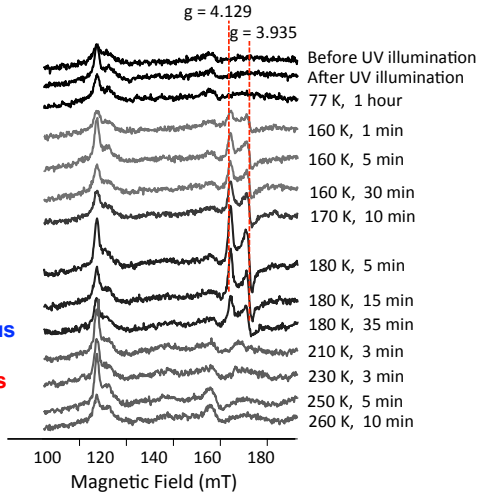
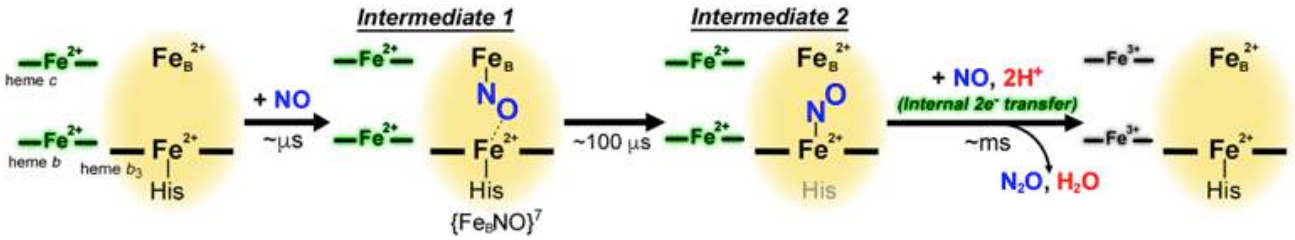


Figure 3 (left) ^{14}NO-^{15}NO Difference IR spectrum of Intermediate I (300 μs) (*unpublished result)*

Figure 4 (right) ESR Spectral Changes of NOR in the Cryo-photolysis and Annealing (*unpublished result)*



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意義と波及効果：酵素反応では短寿命の反応中間体が存在し、それを**励起状態**と捉える事ができ、これにより酵素反応の特異性と高活性を特徴づけている。反応中間体の構造と電子状態を知る事により、その反応機構の詳細を理解できる。本研究では、一酸化窒素還元反応を取り上げて、caged NO 化合物の**励起**を活用した時分割反応・分光解析により、その触媒反応の素反応速度の解析ならびに酵素反応中に現れる短寿命反応中間体の構造・電子状態解析をおこなった。Caged 化合物が従来、細胞生物学などで用いられてきたが、本研究により反応中間体解析に使える事を示せた。将来的には、短寿命反応中間体の X 線結晶構造解析に適用したい。

[Category 3]

Production of molecular ions at 0.4 K in helium nanodroplets and its application to molecular approach to the superfluid interface

（ヘリウムナノ液滴を用いた極低温分子イオン生成と超流動界面への分子論的アプローチ）

T. Azuma[1], A. Iguchi[1,2], S. Kuma[1], Y. Nakano[3], H. Tanuma[2]
[1]AMO Physics Laboratory, RIKEN,
[2]Department of Physics, Tokyo Metropolitan University
[3]Department of Physics, Rikkyo University

Helium droplets are nano-scale, superfluid clusters of liquid helium at a temperature of 0.4 K. Their capability of capturing atomic and molecular impurities enables us to study the atomic/molecular scale interactions between matter and superfluid. Since helium droplets are produced in a molecular beam, various established experimental techniques of laser spectroscopy and mass spectrometry are applicable to the droplet system. At this low temperature, the captured molecule is in the ground state of their vibrational motions and a very limited number of the rotational states are populated. This is also true for large molecules and molecular cluster systems, which are still difficult targets to prepare at cryogenic temperature in their isolated form. Due to superfluidity of helium droplets, the molecule behaves as a free rotator like in the gas phase, but with modified moments of inertia for the rotational motion. In this study, we apply the helium droplet technique to molecular ions to explore the microscopic interface between the impurity and the superfluid in this highly heterogenetic system. The control of a helium droplet beam by electrostatic fields allows us to observe the slow temperature change of the droplet over seconds by injecting into our cryogenic ion storage ring RICE. Our droplet source is operating with the optimized setup for this study [1].

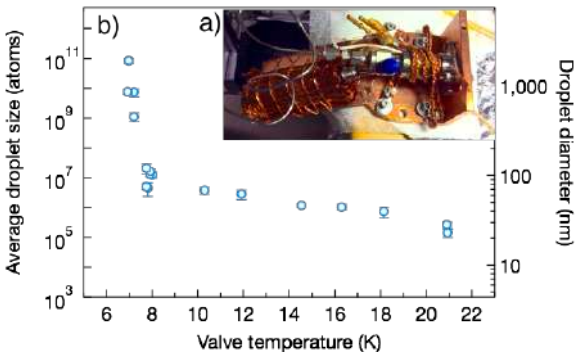

Figure 1 Development of a pulsed source of extremely large helium droplets. (a) A modified commercial valve. (b) Valve temperature dependence of the droplet size. Micron-size superfluid droplets are available to prepare a large system of molecular ions at a temperature of 0.4 K.

To prepare cold molecular ions in this study, we adopted photoionization of pre-captured neutral molecules, because the direct pickup of molecular ions by the droplets has a disadvantage in producing a large number of bare ions in the pick-up stage. To improve the photoionization efficiency, we utilized the resonance-enhanced multiphoton ionization (REMPI) method. Here we chose as our sample aniline ($C_6H_5NH_2$), which is a simple aromatic amine. An aniline vapor was introduced into a small cell in the droplet chamber via a gas line from a room temperature liquid of aniline. After the pick-up, aniline aggregates quickly dissipating their binding energy in the clustering process by evaporation of He atoms from the droplet surface. At the downstream of the beam, we irradiated a UV laser light at 295 nm, which is resonant to the $S_1 \leftarrow S_0$ electronic transition of neutral aniline molecules. After photoionization, the resulting ions were mass-analyzed using a time-of-flight spectrometer.

Figure 2 is a typical mass spectrum measured by REMPI in this study. In addition to the aniline monomer peak at m/q = 93, we observed the (aniline-He$_n$)$^+$ peaks where n is the number of He atoms attached to the monomer.

Although the exact structure of the (aniline-He$_n$)$^+$ cluster is unknown, we speculate that several layers of He atoms surround the aniline cation core when n is large. The binding energy of a He atom to an aniline cation is expected to be small, particularly being a few Kelvins in temperature if the He atom locates in the outmost layer. Thus, the existence of the large clusters in the spectra is a firm evidence of the internally cold ions.

Furthermore, we observed pure aniline cluster ions consisting of up to 14 aniline units as shown in Fig. 3, measured under a different condition from Fig. 2. Here, the initial droplet size is estimated to be 10^6 He atoms/droplet. These clusters were first prepared in their neutral forms in helium droplets. After picked up by a droplet, neutral monomers aggregated via the van der Waals interaction. In the REMPI process, the excess energy of ionization is removed by surrounding He atoms, and the cationic clusters are stabilized. The existence of such large organic clusters after photoionization is an outstanding characteristic of the helium droplet technique. Generation of larger clusters is possible by optimizing the droplet size and the initial neutral cluster size, which open a way to study complex molecular systems and their inherent intermolecular interaction under frozen condition at a cryogenic temperature.

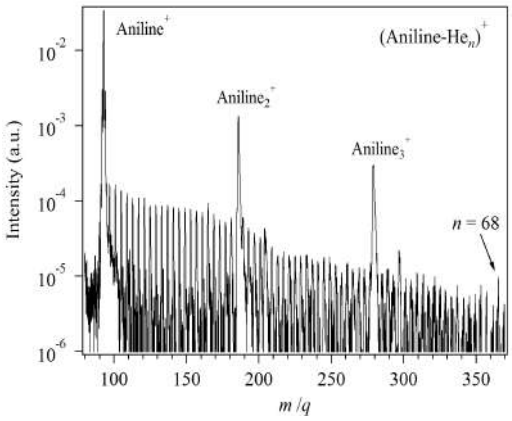

Figure 2 Mass spectrum of cations of aniline and its clusters with He atoms.

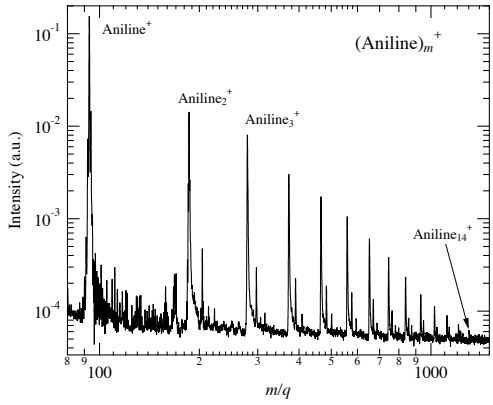

Figure 3 Mass spectrum of cations of aniline cation clusters produced in helium droplets.

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意義と波及効果：低温で顕著に現れる物質の量子性を研究する上で、物質の構成単位である分子を対象とする時、特にそのサイズが大きい場合は振動・回転の内部自由度を冷却することが現状の実験技術では困難である。温度 0.4 K のヘリウム液滴を用いてその内部に分子イオンを生成することで、分子サイズに関わらず非常に短い時間で内部自由度を冷却することが可能となる。我々は研究室で開発したパルス巨大ヘリウム液滴ビームを用いて、まず 0.4 K まで冷却された中性アニリン分子を、電子遷移に共鳴するレーザー光を用いて選択的に光イオン化することに成功した。また液滴への分子捕捉過程を制御することにより 0.4 K 液滴内部に中性アニリンクラスターを初めに生成し、光イオン化法で**極低温クラスターイオンが効率よく生成**されることを見出した。この手法により、これまで単離生成することが困難であった大サイズ分子のクラスターイオンの研究が可能となり、複雑且つ多様な分子ネットワークを形成する分子間相互作用の検出への展開が期待される。またこのイオン内包液滴を我々の極低温イオン貯蔵リング RICE と組み合わせることにより、**超流動との境界面**を通した分子スケールでの超流動ダイナミクスの探求が可能となる。

[Category 3]

Control of the electrical conductivity in diamond by heavy-ion implantation: An application of atomic-scale interface to device technology

（ダイヤモンド電気伝導の制御：原子スケール界面のデバイス工学への応用として）

Hiroki Yamazaki,[1] Takaaki Minamidate,[2] Masanori Kidera,[3] Ayako Yamamoto,[4] Reizo Kato,[2] and Hideki Ueno[1]

Nuclear Spectroscopy Laboratory, RIKEN, [1] Condensed Molecular Materials Laboratory, RIKEN, [2] Ion Source Team, RIKEN Nishina Center, [3] Graduate School of Engineering and Science, Shibaura Institute of Technology [4]

Diamond is an excellent electrical insulator with a large band-gap of 5.5 eV. Interestingly, it becomes a semiconductor when doped with a small amount of boron (for *p*-type) or phosphorus (for *n*-type). Ekimov *et al*. reported that boron-doped diamond, when doped beyond the metal-to-insulator transition at $n_B \sim 3\times10^{20}$ B/cm^3, shows superconductivity in the samples grown by the high-pressure and high-temperature synthesis.[1] Theoretically, the superconducting critical temperature T_c can be raised substantially by reducing the effects of disorder in the boron-doping processes.[2] For a higher T_c, more subtle control of doping using CVD and/or MBE methods is highly required, whereas a different method based on ion implantation is also worth investigating since it enables selective ion-doping in a controlled manner, which has great potential for future device applications.

We tried to control the electrical conductivity in diamond by means of the ion-implantation technique, utilizing RILAC at the RIKEN facility. In our study, for *n*- and *p*-type semiconductors (and possibly superconductors), nitrogen and boron ions are implanted into the diamond, respectively. By changing the beam intensity and irradiation time, the concentration of nitrogen or boron was controlled. Note that the *n*-type semiconductor, and needless to say the *n*-type superconductor, achieved by nitrogen doping of diamond is challenging, since nitrogen behaves as a deep donor in diamond and does not contribute to conductivity.[3] The electrical conductivity observed in the nitrogen-implanted diamonds (e.g., at $n_N \sim 7.5\times10^{21}$ N/cm^3) is, therefore, most likely explained in terms of the carbon atoms connected via the sp^2 bonding produced by radiation damage. The Raman spectroscopy supports this scenario.

In this fiscal year, we have mainly investigated boron-implanted diamonds. A boron beam was implanted at 5 keV using an ECR ion source. We thus prepared ten samples of different concentrations from $n_B \sim 4.9\times10^{20}$ to 6.8×10^{22} B/cm^3. In order to detect the appearance of superconductivity, the static magnetization

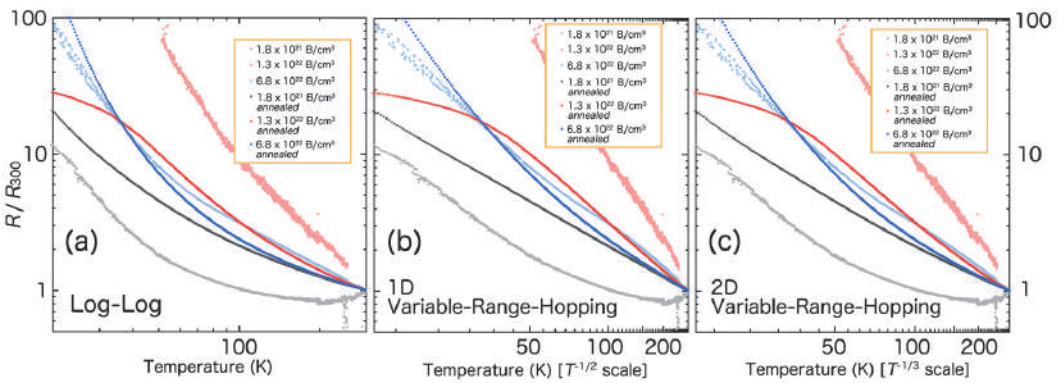

Figure 1 Temperature dependence of electrical resistivity before and after annealing for the B concentrations of n_B~1.8×10^{21}, 1.3×10^{22} and 6.8×10^{22} B/cm^3

measurements were carried out using MPMS (Quantum Design). The electrical resistance was also measured by the four-probe DC method to confirm superconductivity. The results of these measurements show that the as-implanted diamonds do not exhibit superconducting transitions at low temperatures even though the doping concentrations are nominally beyond the metal-to-insulator transition at $n_B \sim 3\times10^{20}$ B/cm^3. Examples of the typical temperature dependence of electrical resistivity are shown in Fig. 1 for the samples of $n_B \sim 1.8\times10^{21}$, 1.3×10^{22} and 6.8×10^{22} B/cm^3.

We tried annealing treatments after implantation in order to reduce the lattice damage produced possibly during the ion implantation. As the phase diagram of carbon (Fig. 2) shows, diamond is not stable at low pressures; we annealed the samples at 800°C and 4 GPa (in the diamond-stable region) for one hour. The annealed samples, however, indicate no sign of superconductivity (see Fig. 1). The annealing treatments rather degraded the diamond crystals: the (222) peak at a higher angle in X-ray diffraction measurement has disappeared after annealing, whereas the (111) peak remains. Figure 3 shows a typical change in the Raman spectra (632.8 nm excitation) after annealing. Though the intense peak for the sp^3 bonding remains prominent in the spectra, the fluorescence emission due to NV$^-$ (negatively charged nitrogen-vacancy) defect centers becomes obvious at ZPL (zero-phonon line) and *n*PLs (*n*-phonon lines; "phonon side band"). This change suggests that the annealing treatment promotes the NV formation process, where nitrogen ions have been embedded in the Ib-type diamonds as impurities before the ion implantation. Hereafter, we also have to consider the effect of the NV$^-$ centers on the electrical conductivity in the implanted diamonds. We are preparing for the boron implantation of the IIa-type diamonds with the nitrogen concentration less than 8 ppm. We hope the high purity diamonds resolve the problem of the NV formation. Lastly, the mechanism of the electrical conductivity in the implanted diamonds is discussed shortly from the point of view based on the temperature dependence of the electrical resistivity. In order to confirm the power-law dependence on temperature, Fig. 1 (b) and (c) show the $T^{-1/2}$ and $T^{-1/3}$ plot, respectively. We cannot positively assert that these plots are the evidence of 'hopping conductivity'; they do not contradict with the hopping conductivity in carrier-doped semiconductors, however.

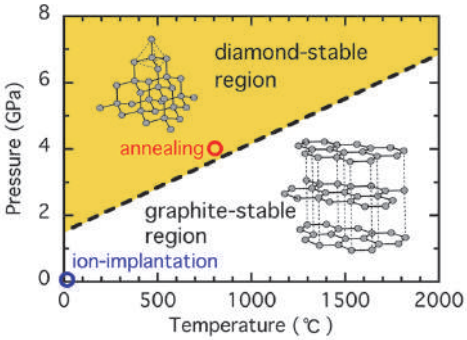

Figure 2 The phase diagram of carbon.

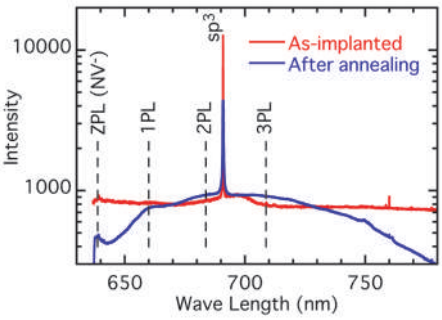

Figure 3 Typical laser Raman spectra for n_B~6.8×10^{22} B/cm^3.

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意義と波及効果：本課題では、物質科学研究と実験核物理研究の双方の研究者による共同研究により、未だ根本的に解決されてないダイヤモンドへの高濃度ドーピング技術を、重イオンビーム照射による方法により開発しようとするもので、特に CVD 法では実現が困難な n 型ドーピングによる超伝導ダイヤモンドの合成を目指している。双方の専門家が参画することで効果的な研究実施体制を組み、照射と試料の分析が円滑に行われている。まずはホウ素のビームドープによる超伝導の発現が可能な照射及び試料のアニーリングの様々なパラメータの調査を行っているが、残念ながらここまで超伝導の発現が確認されていない。難しい課題ではあるが、成功した場合のインパクトは大きく、分野横断的開拓研究課題にふさわしい課題として引き続き取り組む。

[Category 4]

Electric quadrupole mechanism of vibrational sum frequency generation at air/liquid interfaces

（気液界面における電気四極子機構による振動和周波発生）

Korenobu Matsuzaki[1,2], Satoshi Nihonyanagi[1,3], Shoichi Yamaguchi[1,3], Takashi Nagata[2], and Tahei Tahara[1,3]

[1] Molecular Spectroscopy Laboratory, RIKEN, [2] Department of Chemistry, School of Science, The University of Tokyo, [3] Ultrafast Spectroscopy Research Team, RIKEN Center for Advanced Photonics (RAP)

Sum frequency generation (SFG) is a unique tool that allows us to investigate the molecular-level structure of air/liquid interfaces. The interface-selectivity of SFG is based upon the symmetry of the system under investigation. In the bulk liquid, the inversion symmetry is macroscopically preserved because the molecules are randomly oriented. Meanwhile, the inversion symmetry is broken at the interface where the molecules are oriented in a particular direction due to the asymmetry of the surrounding environment. Based on this symmetry consideration, SFG is used as an interface-specific spectroscopic tool, because it is widely believed that SFG occurs only in the region where the inversion symmetry is broken.

This reasoning, however, is valid only within the electric dipole approximation, and it is no longer correct when the contributions beyond the electric dipole approximation are also taken into consideration. More specifically, if we consider the electric quadrupole contribution, which is the lowest-order contribution beyond the dipole approximation, we can show that SFG occurs even without symmetry breaking and that bulk molecules also contribute to SFG. Thus, the information contained in SFG spectra is strongly dependent on the mechanism with which SFG occurs, and it is crucial to examine the mechanism before interpreting the spectra. In this study, we investigated the electric quadrupole contribution to SFG both theoretically and experimentally. In particular, we propose how we can infer the mechanism of SFG from experimentally obtained spectra, and how the SFG spectra can be interpreted in each case.[1]

From a theoretical side, we formulated the quadrupole contribution to SFG and evaluated its significance. Usually, the quadrupole contribution is believed to be negligible, because the quadrupole transition probability is proportional to the electric field gradient, which is very small in homogeneous media. At the interface, however, a large electric field gradient exists because of the refractive index mismatch between the bonding media. Thus, the electric quadrupole may have a significant contribution to SFG at the interface.

Our quadrupolar theory also predicts which molecules and which vibrational modes appear in SFG spectra when SFG is caused by the quadrupole contribution. The selection rule derived in this way was clearly different from the one derived under the dipole approximation. This difference in the selection rule can be exploited to examine if the experimentally observed SFG spectrum originates from the quadrupole contribution. The flowchart in Fig. 1 explicitly shows how this can be done in practice and how the observed spectra can be interpreted in each case.

As an experimental demonstration, we examined SFG at the air/benzene and air/decane interfaces using heterodyne-detected vibrational SFG spectroscopy.[2, 3] At the air/benzene interface, some of the observed bands were attributed to interfacial molecules, whereas the others were assigned to bulk molecules. This experimental result was in good agreement with the vibrational selection rule of the quadruolar mechanism, and we have therefore concluded that SFG at the air/benzene interface was dominated by the quadrupole

contribution. This result suggests that the benzene molecules preserve their centrosymmetric structure at the interface, in which case SFG is forbidden within the dipole approximation. We note that SFG spectra contain no information about the orientation of interfacial molecules when SFG is due to the quadrupole contribution. At the air/decane interface, on the other hand, all the vibrational bands were assignable to the interfacial molecules. In particular, the bands observed with the PSS polarization combination were also attributable to the interfacial molecules. From these observations, we concluded that the SFG signal observed at this interface occurred predominantly with the dipolar mechanism. This result indicates that the decane molecules have a polar orientation at the air/decane interface, despite their low polarity.

The experimental demonstration here clearly shows that the interpretation of the SFG spectra is strongly dependent upon the mechansim of SFG. Thus, the present work serves as an important guideline to make a correct molecular-level interpretation of experimentally obtained SFG spectra.

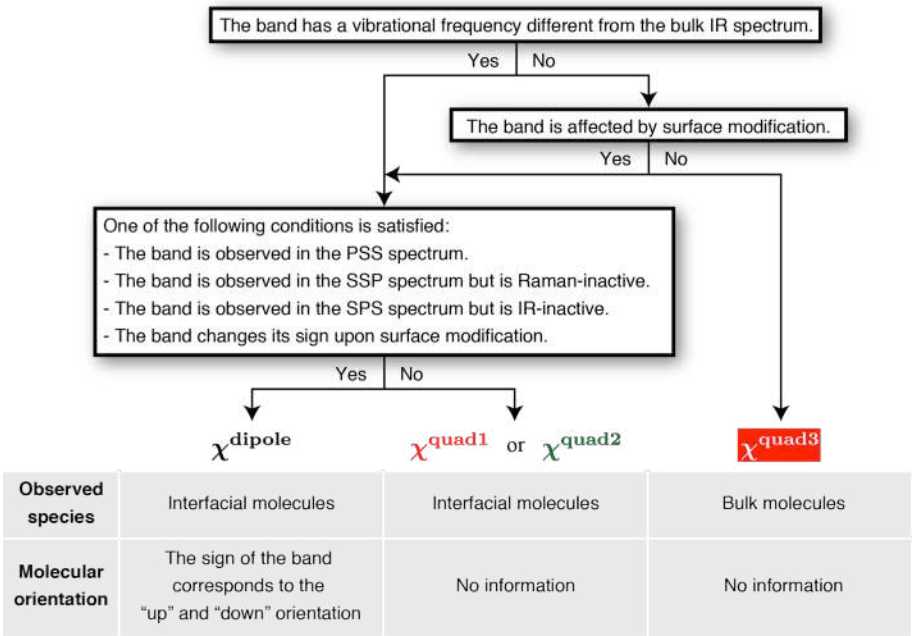

Figure 1 A flowchart showing how a certain band in a vibrational SFG spectrum can be interpreted. "PSS", "SSP", and "SPS" indicate the polarization direction of the beams involved in the SFG process, where the first, second, and third letters correspond to the sum frequency, visible, and infrared light, respectively. Here, χ^{dipole} indicates SFG within the dipole approximation, whereas χ^{quad1}, χ^{quad2}, and χ^{quad3} correspond to SFG with a quadrupole contribution.

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意義と波及効果：振動和周波発生分光法は、分子レベルで界面の構造を明らかにするための強力な手法である。通常、実験的に得られる振動和周波発生スペクトルは、電気双極子近似が成り立っていることを前提として解釈される。しかし実際には、より高次の寄与である電気四極子が関与している場合があり、この場合に電気双極子近似を前提にスペクトルの解釈を行うと誤った結論を導いてしまう。本研究では、実験的に観測された振動和周波発生の過程に電気四極子が関与しているか否かをどのように調べるか、また電気四極子が関与している場合には得られたスペクトルをどのように解釈すべきかについて、理論と実験の両面から明らかにした。

[Category 4,2]

Controlling exciton formation at a single-molecule interface

（単分子界面における励起子形成の制御）

Kensuke Kimura[1, 2], Hiroshi Imada[1], Kuniyuki Miwa[1, 3], Miyabi Imai-Imada[1, 2], Shota Kawahara[1, 2], Jun Takeya[2], Maki Kawai[4], Michael Galperin[3], and Yousoo Kim[1]

[1]Surface and Interface Science Laboratory, RIKEN,

[2] Department of Advanced Materials Science, Graduate School of Frontier Science, The University of Tokyo,

[3] Department of Chemistry & Biochemistry, University of California San Diego,

[4] Institute for Molecular Science, National Institutes of Natural Sciences

Exciton formation by charge injection is an essential process in organic light emitting diodes (OLEDs). The injected charges form singlet excitons (S_1) and triplet excitons (T_1) in a 1:3 ratio according to the spin statistics, thus effective utilization of T_1 is the primary strategy for increasing quantum efficiency of OLEDs. T_1 has lower energy than S_1 due to the exchange interaction. The energy difference, in principle, enables selective formation of T_1 at low voltage. Such selective T_1 formation would realize low driving voltage of OLEDs, which can reduces power consumption and improves device lifetime. However, the way to achieve the selective and direct T_1 formation has not been established yet.

In this work, we demonstrate a simple way for the selective T_1 formation [1] which utilizes a charged state of molecule by the investigation of a single-molecule electroluminescence using a scanning tunneling microscope (STM) [2-5]. We measured scanning tunneling luminescence (STL) and its bias voltage dependence of a 3,4,9,10-perylenetetracarboxylicdianhydride (PTCDA, Fig. 1A) molecule adsorbed on three atomic layer (3ML) thick NaCl film grown on the Ag(111) surface. Only phosphorescence is observed at low applied voltage, which shows that T_1 is selectively created without forming S_1. Based on the differential conductance (dI/dV) measurement reported in the previous paper [6], the selective T_1 formation is explained by spin-selective electron removal from the highest occupied molecular orbital (HOMO) of a negatively charged PTCDA.

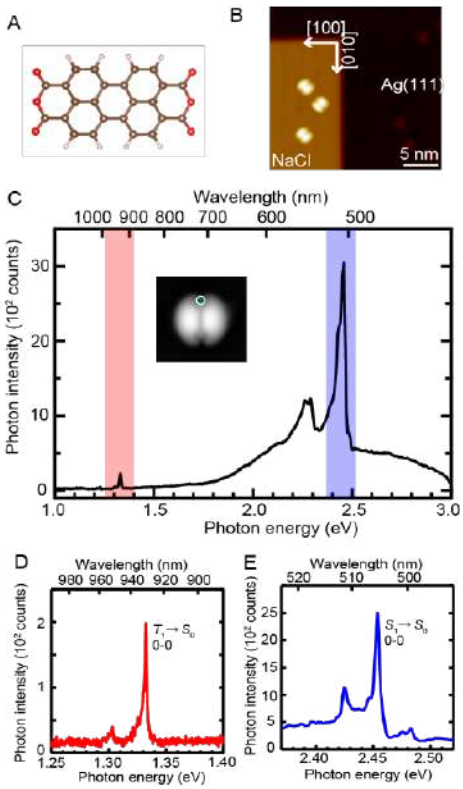

Fig. 1 (**A**) Molecular structure of PTCDA (brown, C; red, O; beige, H). (**B**) An STM image showing two PTCDA molecules on NaCl(3 ML). (25 × 25 nm^2, V = 1.0 V, I = 10 pA). (**C**) An STL spectrum of PTCDA (V = -3.5 V, I = 50 pA, 120 s). (**D-E**) STL spectra (V_s = -3.5 V, I_t = 50 pA, t = 180 s). **D**: energy range: 1.25-1.40 eV (blue region in **C**), and **E**: 2.37–2.52 eV (red region in **C**).

Fig. 1B shows an STM image of PTCDA/NaCl(3ML)/Ag(111) that appear as double-lobe structure with a nodal plane along the long axis of the molecule. The STL spectrum (Fig. 1C) obtained with the tip located on PTCDA shows a broad peak spread from 1.5 eV to 3.0 eV and several sharp peaks around 1.3, 2.25 and 2.4 eV (Fig. 1C). The broad peak is attributed to the radiative decay of the plasmon localized between the STM tip and substrate. To reveal the detail structures of the sharp peaks, STL spectra are measured with higher energy resolution in the range of 1.25-1.40 eV (Fig. 1D) and 2.37-2.52 eV (Fig. 1E). In Fig. 1D, main peak is at

1.33 eV and smaller peaks are around the main peak. Similarly, main peak is at 2.45 eV in Fig. 1E. Based on the good agreement with Time dependent density functional theory (TD-DFT) calculation, the observed main peaks at 1.33 and 2.45 eV are assigned to the phosphorescence and fluorescence, respectively.

To investigate the exciton formation mechanism, we examined the voltage dependence of the photon intensities of phosphorescence and fluorescence as shown in Fig. 2, which clearly show the threshold voltages (V) for phosphorescence and fluorescence at V = -2.1 and -3.3 V, respectively. The threshold voltage difference is 1.2 V, which corresponds to the S_1-T_1 energy difference, 1.12 eV, measured from the STL spectra.

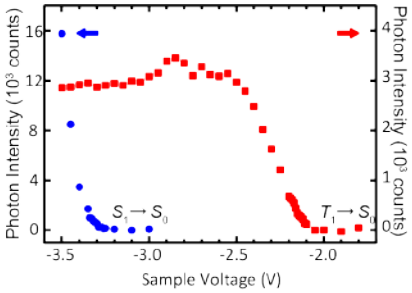

Fig. 2 Sample voltage dependences of the intensities of fluorescence (blue circle) and phosphorescence (red square).

	-1 ↔ S_0	-1 ↔ T_1	-1 ↔ S_1
transition energy	-3.92 eV	-5.30 V	-6.46 V
sample voltage	-0.35 V	-1.73 V	-2.89 V

Table 1 Theoretical analysis for the electron transport through an isolated PTCDA molecule

Based on the previous report [6], PTCDA is expected to be negatively charged on NaCl/Ag(111) due to the high electron affinity of the molecule and low work function of the substrate [7], thus an electron occupies the lowest unoccupied molecular orbital (LUMO). When further voltage is applied, the electron occupying HOMO can be pulled out from the molecule from -1 charged states. Assume that electron removal occurs from the -1 charged state, the two electrons in HOMO have different energies owing to the exchange interaction with the electron in LUMO. If we increase the applied voltage under this situation, the electron in HOMO whose spin is “anti-parallel” to the spin of the electron in LUMO is first pulled out to exclusively form T_1. When further voltage is applied and the removal of the other “parallel-spin” electron from HOMO turns into possible, both T_1 and S_1 are formed. This process can reasonably explain the observations of the voltage dependence of STL.

In this work, we demonstrated selective T_1 formation by spin-selective electron transport through a single molecule. We prepared a charged molecule by tuning the energy level alignment between the LUMO and the Fermi level of the substrate. Various combinations of molecules and substrates are thus available for realizing selective T_1 formation, which would propose diverse ways of developing OLEDs with higher energy efficiency.

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意義と波及効果：本研究では STM 発光分光装置を用いて、単分子**界面**における分子の発光特性を調べることで、三重項励起子を選択的に形成できることを示した。その要は、不対電子が分子中に存在することで生じる交換**相互作用**であり、そのような有機 EL デバイスを設計・開発すればエネルギー効率が高いデバイスが作製できることを示している。さらには、三重項励起子を低電圧で形成できることから材料選択の幅が広がり、これまで実現できなかった青色のりん光材料を実現できる可能性がある。単一分子発光測定という基礎研究で得られた発見であるが、有機 EL デバイスへの応用研究に新たな知見を与えられると期待できる。

[Category 4]

Iron Dynamics (Reduction, Transport and Sensing) on Biological Membrane-Protein Interface

（細胞膜とタンパク質の界面における生体内鉄動態解析）

Hitomi Sawai, Yoshitsugu Shiro[1], Yudai Nishitani[1], Michiyo Takahara[1], Hiro Nakamura[2], Tamao Hisano[2] and Hiroshi Sugimoto[3]

[1]Cellular Regulation Laboratory, University of Hyogo, [2]RIKEN BDR, [3]RIKEN RSC

Iron is one of essential elements for all of living system containing microorganisms, plants and animals. It usually acts as an active site of proteins/enzymes, thus being involved in many physiological actions through chemical reactions such as electron transfer, oxidation-reduction, ligand binding and so on. Iron and iron compound are transported from dietary foods to cell across cellular membrane, in which membrane-integrated proteins works. We have been studying structure and function of such membrane-proteins involved in the iron absorption into cell.

1. Human Duodenal Iron Reductase

In human, iron in dietary foods is absorbed at duodenum and small intestine. In this case, ferric iron (Fe^{3+}) must be reduced to ferrous iron (Fe^{2+}) by duodenal iron reductase (Dcyt*b*), and then is transported into the duodenal cell through divalent metal transporter (DMT1). Dcyt*b*, which is membrane-integrated protein present in the duodenum cell membrane, reduces the ferric iron outside the duodenum cell with electrons which are supplied from ascorbic acid inside the cell, indicated that this protein mediates electron transfer across the cellular membrane. We successfully determined the crystal structure of human Dcyt*b* (Figure 1). On the basis of the structural information, we could identify amino acid residues involved in the iron-binding, ascorbate-binding and intra-molecular electron transfer.

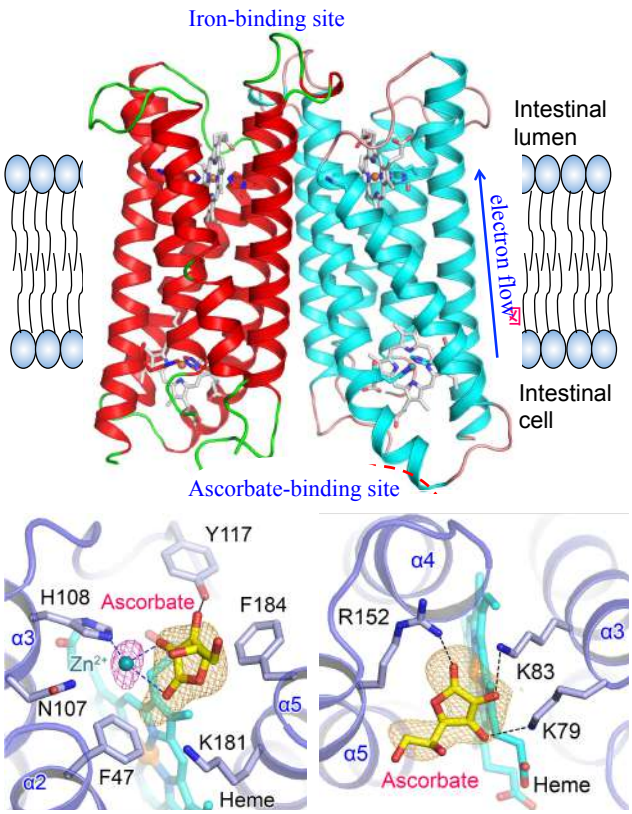
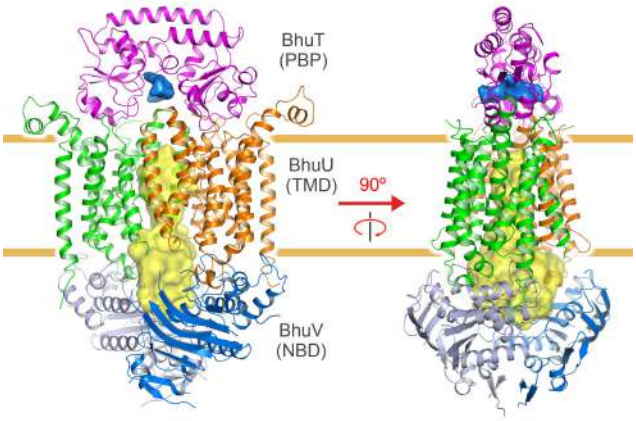


Figure 1. Overall structure of Dcytb, its metal-binding and ascorbate-binding structures

2. Pathogenic Iron Importer/ Heme Sensor Protein

Pathogenic bacteria get iron from heme (iron-porphyrin compound) of hemoglobin in red blood cell of host, and use it for its infection and proliferation. The heme acquisition is conducted by heme importer, which is present in the bacterial cellular membrane. We successfully determined structure of pathogenic heme importer by the X-ray crystallography, as shown in Figure 2. This is the structure in the inward form, in which the heme transporting channel is opened toward the inside of the cell. The structural information was provided



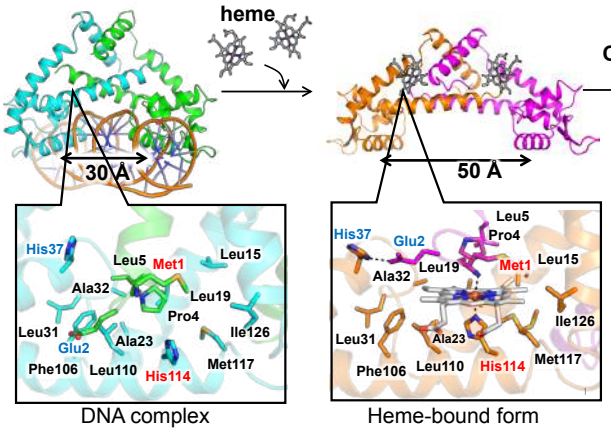


Figure 3 (left). Structures of bacterial heme importer

Figure 4 (right). Structures of heme sensor protein in DNA-bound form and heme-bound form

to the molecular dynamic simulation, which showed dynamic conformational change of this transporter during the heme translocation. In addition, we are now trying to determine the outward structure of the heme importer by the CryoEM technique.

However, since excess amount of heme imported in the cell is toxic even for pathogen, due to generation of reactive oxygen species, pathogenic bacteria expresses heme exporter, in response to the heme concentration monitored by heme sensor proteins. In Figure 3, the structures of the heme sensor protein are illustrated in the heme-bound and DNA-bound forms, showing recognition mechanism of the heme and of DNA by the sensor protein. The structural comparison indicated how the heme binding changes the protein conformation for dissociation from DNA, allowing us to propose the heme sensing mechanism by the sensor protein. Upon the dissociation of the heme sensor protein from DNA, the expression of the heme exporter can be facilitated. Structural determination of the heme exporter is now underway.

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意義と波及効果：鉄は生命現象において必須の元素であり、その動態（吸収、輸送、感知、貯蔵など）の中で鉄の膜輸送は生体膜**界面**で行われ、膜に存在する様々なタンパク質がそれに寄与している。本研究では、ヒトと病原菌における鉄輸送に関わる膜タンパク質の構造と機能を明らかにした。これにより、生体における鉄の吸収を、細胞膜界面での現象として分子・原子レベルで理解する道が拓けた。加えて、近年注目を集めている、低温電子顕微鏡法を使った膜タンパク質の構造解析にも成功しており、今後、生体膜界面での鉄吸収をより幅広く理解できる手法を獲得した。

[Category 4]

Singular interfacial phenomenon of DNA brush and its applications for biosensing

（DNA ブラシが示す奇妙な界面現象の解明とバイオセンサーへの応用）

Masahiro Fujita[1], Yoshifumi Sakamoto[1], Surachada Chuaychob[1,2], Rodtichoti Wannapob[1], and Mizuo Maeda[1,2]

[1] Bioengineering Laboratory, RIKEN CPR, [2] Graduate School of Frontier Sciences, The University of Tokyo

Gold nanoparticles (AuNPs) functionalized with single-stranded DNA (ssDNA) show a high colloidal stability. The hybridization with a target DNA sequence induces a DNA-linked particle aggregation, in which the DNA duplex crosslinks the particles. The color change from red to blue due to surface plasmon shift occurs. On the other hand, our group reported another aggregation behavior, called non-crosslinking aggregation, which is caused by a change in the physical properties of the particle surfaces.[1,2] A high colloidal stability of AuNP with ssDNA is due to their electrostatic and steric repulsions, ascribed to the negatively charged and flexible DNA strands. The hybridization to their fully complementary DNA targets (in sequence as well as in chain length), however, causes the particles to aggregate. The decrease of entropic effect by switching from flexible ssDNA to rigid double-stranded DNA (dsDNA) is likely responsible for this type of aggregation, in addition to the salt screening. This is in contrast with the DNA-linked particle aggregation. Interestingly, the particles remained dispersed after the hybridization with one base-mismatched DNA (msDNA). The molecular motion due to unpairing at the terminal base is considered to contribute to the colloidal stability.[3] This singular interfacial phenomenon is thus expected to be useful for the simple and rapid detection of single-base mutations.

With the aim of further understanding the mechanism, we tried to apply an external interaction in the system of DNA-functionalized AuNPs. The addition of polyethylene glycol (PEG) to the colloidal system causes the attractive interaction between the particles, called as depletion effect. Because the depletion effect increases with increasing the concentration of crowding agent, desired attractive interaction between the particles can be tuned by adjusting PEG concentration. The PEG concentration necessary to the non-crosslinking aggregation was founded to depend on the DNA structures. (Figure 1) AuNPs with dsDNA

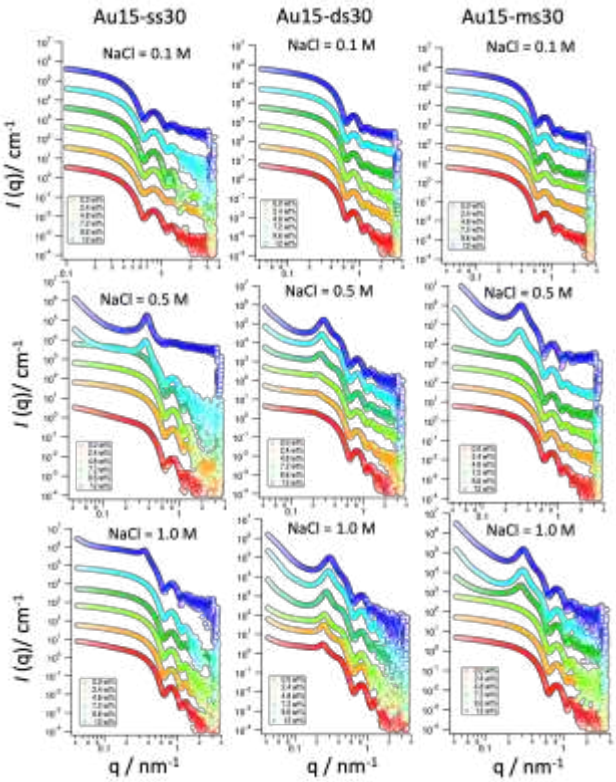

Figure 1 SAXS profiles of DNA-functionalized AuNPs at [NaCl] = 0.1, 0.5 and 1.0 M, varying PEG concentrations (0 to 12 wt%). AuNPs with 15 nm in diameter were functionalized with 30-mer ssDNA, dsDNA and msDNA. The interference peaks, indicating the non-crosslinking aggregation, were observed at certain PEG concentrations.

aggregated at the lowest concentration. Noteworthy, AuNPs with msDNA showed a high stability similarly to those with ssDNA, meaning that the entropic repulsion due to one base unpairing is comparable to the steric effect due to the flexibility of ssDNA. As PEG concentration further increased, the particles packed more closely. Even for dsDNA, the distance between the particles steadily decreased with increasing in depletion attraction, in contrast to the case of crosslinking aggregation. This fact proved that the particle aggregation of AuNPs-DNA is not facilitated by the base stacking attraction between the blunt ends of dsDNA. The difference in entropic effect due to the flexibility and motion of DNA strands accounts for the DNA structural dependency of colloidal stability.

On the basis of the above experimental facts, we assumed that the change in DNA structure is a key role for non-crosslinking aggregation. Other DNA conformational transitions could also induce the change of colloidal stability. Here, we focused on G-quadruplex (G4) DNA (Figs. 2A – 2C). The highly polymorphic G4s are an outstanding candidate because the conformational change is expected to occur in response to binding with specific target molecules. We prepared various G4 DNA-functionalized AuNPs (G4-AuNPs) and examined the colloidal stabilities. Furthermore, the colloidal system was attempted to apply for biosensing applications.[4]

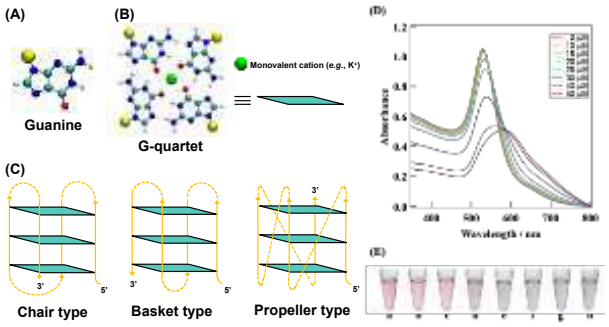

Figure 2 Structures of G4 DNA (A - C) and cisplatin detection using G4-AuNPs (D and E). The panels of (D) and (E) are UV-Vis profiles and corresponding images of G4-AuNPs varying with the concentration of cisplatin.

In this study, we aimed to detect a hazardous small molecule, cisplatin. The colloidal solution color changed in a short time from red to purple-blue after cisplatin was added to the system. The plasmon absorption peak shifted arising from the aggregation, that is, the degree of color change (Figs. 2D and 2E). The binding of cisplatin to G4-DNA led to unfolding G4 conformation. The adduct formation probably caused a reduction in steric repulsion, associated with the unfolding. This induced the non-crosslinking aggregation of particles. The response of color change to cisplatin was found to be faster than those for other analogs such as carboplatin and oxaliplatin, indicating that this system has a high specificity for cisplatin detection. Our nano-biosensor based on G4-AuNPs could be a good candidate to apply in various applications, especially biosensor and medical diagnosis.

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意義と波及効果： DNA 担持ナノ粒子のコロイド分散安定性は DNA 構造に鋭敏に応答する。粒子の分散安定性が変化し、系の色調変化もたらすことから、簡便な遺伝子診断ツールとしての応用展開が期待されてきた。ここでは DNA 担持ナノ粒子が示すこの界面現象のメカニズムを理解するために、構造科学的知見から解明を試みてきた。DNA 鎖の自由度（運動性）に由来するエントロピー反発の差異が特異な界面現象を支配する重要な因子と考えられる。この考えに基づき、DNA 担持ナノ粒子のバイオセンサーとしての応用を進めている。その一環として、四重鎖 DNA で修飾したナノ粒子を作製し、低分子化合物を特異的に検出する系の構築に成功した。様々な物質検出を可能とする DNA 担持ナノ粒子の開発指針を与えるものである。

[Category 5]

Dark-to-bright exciton conversion process for emission enhancement using device interfaces

（デバイス界面における暗い励起子から明るい励起子への変換による発光増強）

Akihiro Ishii[1,2], Hidenori Machiya[1,3], and Yuichiro K. Kato[1,2]

[1]Nanoscale Quantum Photonics Laboratory, RIKEN Cluster for Pioneering Research,

[2]Quantum Optoelectronics Research Team, RIKEN Center for Advanced Photonics,

[3]Department of Electrical Engineering, The University of Tokyo

Atomically thin semiconductors, such as transition-metal dichalcogenides and carbon nanotubes, offer new opportunities for developing nanoscale photonic and optoelectronic devices. The optical processes in these materials are governed by tightly bound electron-hole pairs, or excitons. Interestingly, unexpected optical phenomena can arise from dark states of the excitons, where optical transition is forbidden by the selection rules. Despite their importance, the dark excitons lack spectral signatures and generally their contribution to emission intensity is insignificant. Here, we report that a considerable fraction of light emission can originate from the dark excitons in carbon nanotubes (Figure 1).

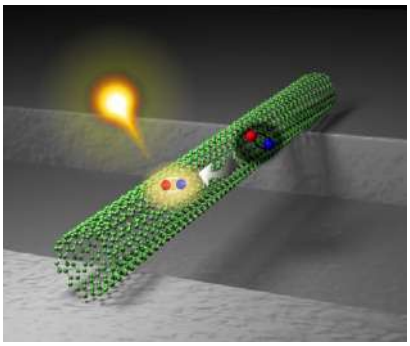

Figure 1 Schematic image of exciton conversion from dark state to bright state.

We perform time-resolved photoluminescence (PL) measurements on individual air-suspended carbon nanotubes to investigate exciton decay dynamics [1]. Figure 2(a) shows a PL decay curve taken from a 4.8-μm-long nanotube with the chirality (11,7). The decay curve shows two components with different lifetimes, and a fit is done with a bi-exponential function convoluted with the instrument response function (IRF). The conversion kinetics can be understood by analyzing the bi-exponential decay curve with a three-level model, which is schematically shown in Figure 2(b). By solving the kinetic equations, we obtain $\tau_{\mathrm{B}} = 69$ ps and $\tau_{\mathrm{D}} = 2422$ ps as well as $\tau_{\mathrm{BD}} = 2369$ ps. The conversion efficiency from dark state to bright state is given by $\tau_{\mathrm{D}}/(\tau_{\mathrm{D}} + \tau_{\mathrm{BD}}) = 51\%$, showing that more than half of the dark excitons are converted to the bright excitons.

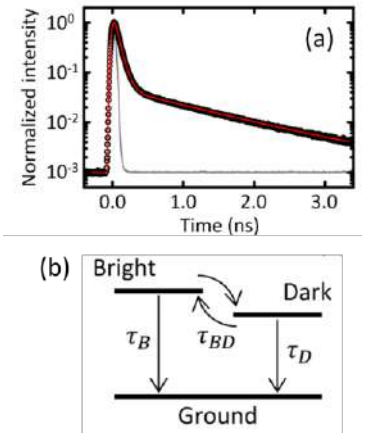

Figure 2 (a) PL decay curve of a.4.8-μm-long air-suspended carbon nanotubes. The gray line represents the IRF, and the red curve is the biexponential fit. (b) Schematic of the three-level model for exciton decay dynamics. τ_{B} and τ_{D} are the effective decay lifetimes for bright and dark states, respectively, and τ_{BD} is the state-transition time between the bright and dark states.

It turns out that the dark-to-bright conversion efficiency depends strongly on the suspended length. We select (9,8) nanotubes with lengths ranging from 0.5 to 4.2 μm and measure PL decay curves. In Figure 3, the PL decay curves taken at various suspended lengths are shown, where drastic changes are observed. As nanotube length becomes longer, decay lifetimes of both fast and slow components become longer, and the intensity fraction of

the slow component increases. The length dependence of the effective lifetimes is analyzed with a random walk theory [2], and we obtain intrinsic lifetimes and diffusion lengths of bright excitons as well as diffusion coefficients for both bright and dark excitons.

Finally we discuss the transition rate between the bright and dark states. In Figure 4, representative values of τ_{BD} for each chirality are plotted as a function of tube diameter d, and a clear family pattern on top of a decreasing trend with tube diameter is observed. The chirality dependence of the bright-dark transition rate is likely related to the bright-dark energy separation ΔE, where a similar family pattern is known with a leading order dependence of $\Delta E \propto 1/d^2$. As the state transition requires a parity flip process, it should be possible to control the conversion efficiency by modifying the exciton scattering site density. We compare the state transition time for a nanotube with and without molecular adsorption. The PL decay curves are taken before and after molecular desorption, and we observe a drastic change of the state transition rate where τ_{BD} increases by a factor of 2 (green triangles in Figure 4), suggesting an enhanced parity-flip process originating from the adsorbed molecules.

The unique nature of the dark states can potentially be utilized to achieve significant performance improvement of nanotube single-photon emitters [3], where not only the brightness can be enhanced by the high conversion efficiency but also the single-photon purity should be improved by the extraordinarily long diffusion length. Our findings also show the nontrivial significance of the dark excitons on the emission kinetics in low-dimensional materials and demonstrate the potential for engineering the dark-to-bright conversion process by using surface interactions. Manipulation of multiple exciton species could lead to the development of advanced devices with devoted channels for exciton transport, recombination, and dissociation.

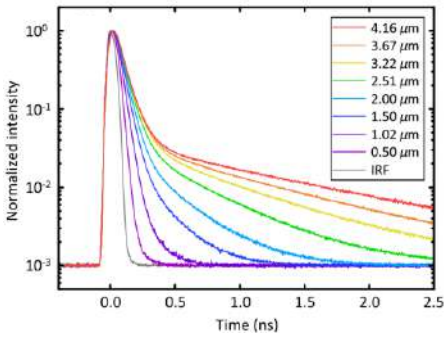

Figure 3 PL decay curves measured from (9,8) nanotubes with various lengths ranging from 0.50 to 4.16 μm. The gray line is the IRF

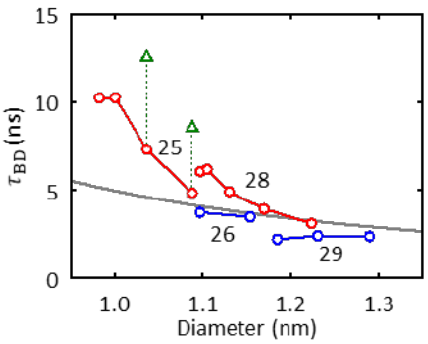

Figure 4 Diameter dependence of state transition time. The data are taken from tubes longer than 2.5 μm. Chiralities with the same family number are connected, and the family numbers are displayed. Red and blue circles correspond to chiralities which belong to type 1 and type 2, respectively. Gray line is a fit described in the text. Green triangles are obtained from molecular desorbed state of (9,7) and (10,5) nanotubes.

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意義と波及効果：カーボンナノチューブは、室温で通信波長帯の単一光子を発生できるため、小型化や長距離伝送に向いており、量子通信への応用が注目されている。本研究では、カーボンナノチューブにおける暗い励起子から明るい励起子への変換効率を定量的に求めることに成功し、変換効率は長いナノチューブほど高くなることを明らかにした。さらに、明るい励起子へ変換される速度はカイラリティ（幾何構造）に依存すること、暗い励起子の 50%以上を明るい励起子に変換できることを実験的に示した。本成果は、カーボンナノチューブの発光効率向上やカーボンナノチューブ単一光子源の性能向上につながると期待できる。

[Category 5, 1]

Determination of ground state phase diagram of an organic Mott-insulator using field effect device interfaces

（電界効果デバイスを用いたモット絶縁体界面の基底状態相図決定）

Hiroshi M. Yamamoto[1], Masayuki Suda[1], Genta Kawaguchi[1], Yoshitaka Kawasugi[2], Kazuhiro Seki[3], Seiji Yunoki[3], and Reizo Kato[2]

[1] Research Center of Integrated Molecular Systems, Institute for Molecular Science, [2] Condensed Molecular Materials Laboratory, RIKEN, [3] Computational Condensed Matter Physics Laboratory, RIKEN

Electron correlation in solid state is a cause of many phase transitions including high temperature superconductivity. Mott-insulator is known as a typical strongly correlated material, whose band-filling is exactly half to enhance the effect of Coulomb interaction. In case of cuprate superconductors, the band-filling has been the major control parameter to tune the strength of electron correlation and thus to induce superconductivity. On the other hand, the band-width has been altered by physical and/or chemical pressures in molecule-based Mott-insulators such as A_3C_{60} and BEDT-TTF cation radical salts in order to obtain superconducting phase. However, it has been difficult to control these two parameters simultaneously in a single compound because the crystal lattice for cuprate is too hard to be compressed adequately enough to reach pressure-induced superconducting phase while the carriers in molecular Mott-insulators are too sensitive to the random energy potential provided by chemical dopants which prevents one to obtain doping-induced superconductivity (Figure 1). Despite these difficulties, it has been theoretically predicted that the band-width-controlled and band-filling-controlled superconductivity should be connected to one another in the ground state phase diagram. Recently, it has been found that field effect device can tune the carrier density considerably if one utilizes high-k gate dielectric or electric double layer. Since the molecular Mott-insulators have both low carrier density and soft crystal lattice, they may provide an indispensable opportunity to investigate the phase diagram of a Mott-insulator in wide parameter space configured by three important thermodynamic parameters: temperature, band-filling (number of particle), and band-width (pressure).

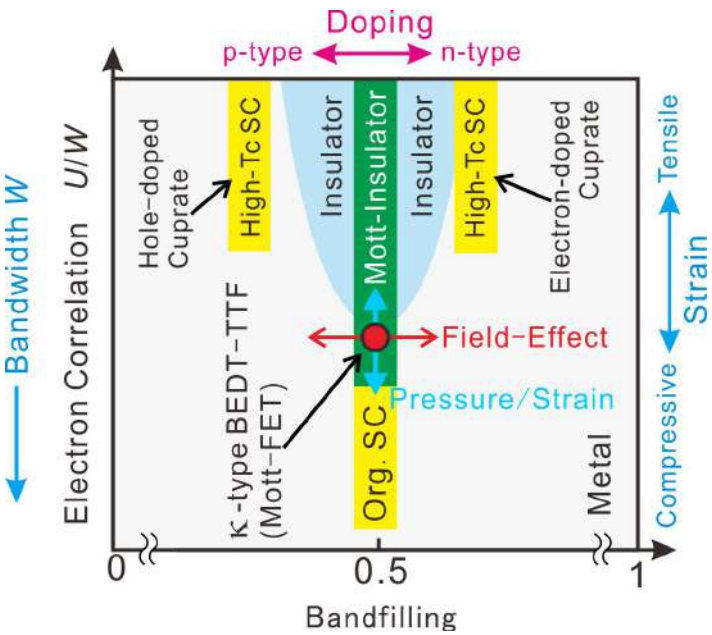

Figure 1 Conceptual ground state phase diagram surrounding a Mott-insulator. The horizontal axis is band-filling, which has been traditionally used for high-Tc cuprates. The vertical axis is band-width that is often used for organic superconductors. SC denotes superconductor, while *U* and *W* denote on-site Coulomb repulsion and band width, respectively.

We demonstrated that the two-dimensional ground state phase diagram of an organic Mott-insulator can be obtained by measuring transport properties under gate electric field and strain effect from the device substrate. In our experiments, FET (field-effect-transistor) or

EDLT (electric-double-layer-transistor) devices were fabricated by using thin single crystal of an organic Mott-insulator κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl (κ-Cl hereafter). In case of EDLT device, a flexible substrate can be used and bended at low temperature. Such a bending can produce strain effect onto the κ-Cl to tune its band-width, while the gate electric field can alter the band-filling. By changing these parameters, a two-dimensional ground state phase diagram has been obtained as shown in Figure 2.[1] This phase diagram clearly shows that both the electron-doped and hole-doped superconductivities are connected to the strain-induced one, which is consistent with the theoretical prediction. At the same time, apparent asymmetry between the electron-doped and hole-doped superconductivities in the parameter space has been revealed. Another FET has been also utilized for fine tuning of the band-filling and band-width of this material, to obtain precise phase diagram in a specific area.[2, 3]

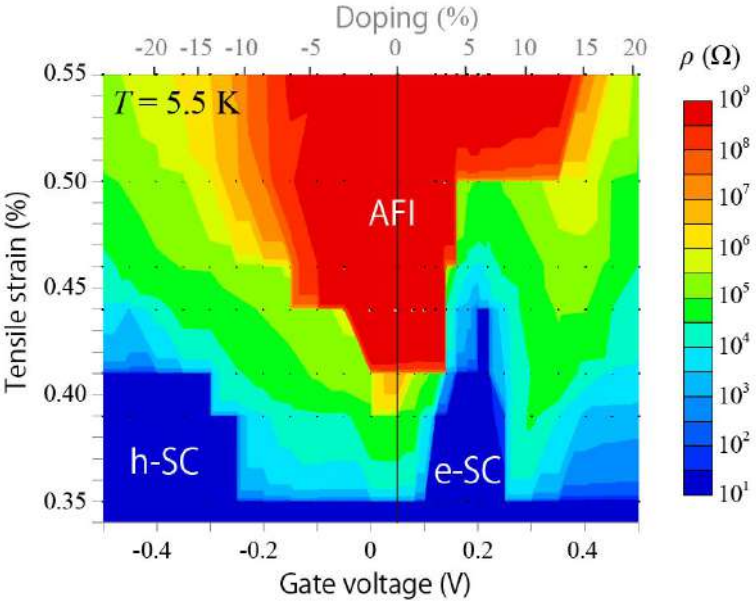

Figure 2 Emergence of both p-type (h-SC) and n-type (e-SC) superconductivity by gate voltage at various tensile strain. The strain is controlling electron correlation U/W while gate voltage controls band-filling (see also Figure 1). AFI denotes antiferromagnetic insulator, meaning Mott-insulating phase.

The above FET is also interesting as an electronic element. Because the metal oxide semiconductor FET (MOS-FET) is known to have several obstacles in further improvements, it is demanded to develop novel devices for next-generation computing, whose concepts and architectures are different from MOS-FETs. Some theoreticians have proposed a phase-switching transistor based on Mott insulators, which can switch its conductance owing to a phase transition by the electrostatic control of carrier density. Although the organic Mott-FET in our experiments does not have efficient ON/OFF properties at room temperature, future development may provide efficient organic Mott-FET working at room temperature.

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意義と波及効果：モット絶縁体は典型的な強相関電子系として知られており、銅酸化物高温超伝導などの興味深い現象はモット絶縁体から金属に転移する際の様々な揺らぎから生じていると信じられている。しかしながら、モット絶縁体の電子相を制御する重要なパラメータである、バンド幅とバンドフィリングを同時に制御する手法はこれまで知られていなかった。有機モット絶縁体は柔軟な結晶格子と低いキャリア密度を有するため、フレキシブルな電界効果デバイスを作製することによって、**デバイス界面**においてこの２つのパラメータを自在に制御し、これまで知られていなかった電子系の相図を決定することが可能となった。これは電子間に働く相互作用の仕組みを解明し、強相関超伝導発現のメカニズムに迫る重要なデータである。また、モット FET は新たな動作原理で動く高効率な電子素子であるため、将来の電子デバイス開発につながる可能性がある。

[Category 5, 1]

Heterointerface-controlled electronic phase transitions in molecular conductors

（ヘテロ界面を利用した分子性導体の電子相制御）

Takaaki Minamidate[1], Yoshitaka Kawasugi[1,2], Hiroshi Yamamoto[3], and Reizo Kato[1]

[1]Condensed Molecular Materials Laboratory, RIKEN, [2]Toho University, [3]Institute for Molecular Science

Mott insulators are materials where one electron localizes on each site due to the strong electron-electron interaction. The superconducting phase in the cuprate-based superconductors and the typical molecular superconductor κ-$(ET)_2X$ (ET = bis(ethylenedithio)tetrathiafulvalene, X: monovalent anion) is located in the vicinity of the antiferromagnetic phase that is a ground state of the Mott insulator. The Mott insulating state is considered to deeply contribute to the mechanism of superconductivity. In order to clarify the relation between the Mott insulating phase and the adjacent superconducting phase, we mainly focused on the thin-film single-crystal of κ-$(ET)_2X$. We have successfully approached the boundary between these two phases using the simultaneous control of the bandwidth and the band-filling.[1,2] As a new target material, we focused on another Mott insulator $EtMe_3P[Pd(dmit)_2]_2$ (dmit = 1,3-dithiole-thione-4,5-dithiolate) with a ground state different from that of κ-$(ET)_2X$.

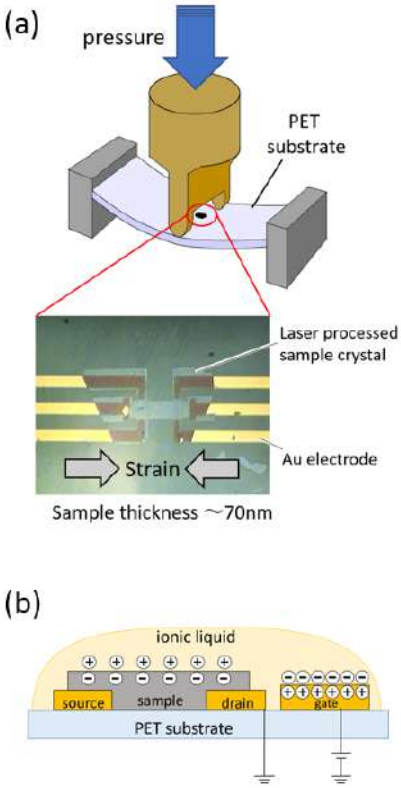

Fig. 1. (a) Setup for uniaxial pressure measurement and picture of the thin crystal of $EtMe_3P[Pd(dmit)_2]_2$ laminated on the PET substrate. (b) Eectric double layer transistor with ionic liquid.

Under ambient pressure, $EtMe_3P[Pd(dmit)_2]_2$ undergoes a transition from a paramagnetic state to a valence-bond order (VBO) phase with lattice modulation at 25 K below which the system exhibits a nonmagnetic state with a spin gap.[3] The VBO phase is suppressed by the application of weak hydrostatic pressure and the superconducting phase appears above 0.4 GPa.[4,5] The relation between the VBO phase and the superconducting phase is not clear yet, and we are interested in comparison with the one between the antiferromagnetic phase and the superconducting phase observed in κ-$(ET)_2X$. Figure 1 shows a setup for the simultaneous control of uniaxial pressure and carrier doping. A single crystal of $EtMe_3P[Pd(dmit)_2]_2$ with a thickness of the several tens of nanometers is laminated on a soft PET (polyethylene terephthalate) substrate, and the center of the substrate is pressed and bended. The sample is compressed along the direction of the bending. The piezo actuator is used to apply the continuous pressure. The carrier doping is accomplished using an electric double layer transistor structure with an ionic liquid. When a positive (negative) gate voltage is applied, electrons (holes) are induced.

Figure 2 shows temperature dependence of the electrical resistances under the uniaxial pressure and carrier-doping in $EtMe_3P[Pd(dmit)_2]_2$. Similar to the hydrostatic-pressure effect, the metallic phase is observed below 25 K in the high uniaxial pressure region. The drop of the electric resistance below 4 K is considered to be a transition toward the superconducting phase, since it disappears under the magnetic field. Applying the gate voltage from the electron-doping region to the hole-doping region, we observed a crossover from the insulating phase to the metallic phase and emergence of the superconducting phase. We also observed an asymmetry in the effects of electron doping and hole doping. Especially, in the electron-doping region, the resistance increases at low temperatures. Although carriers induced in the Mott insulator contribute to electrical conductivity and reduce electrical resistance, we obtained contrary results.

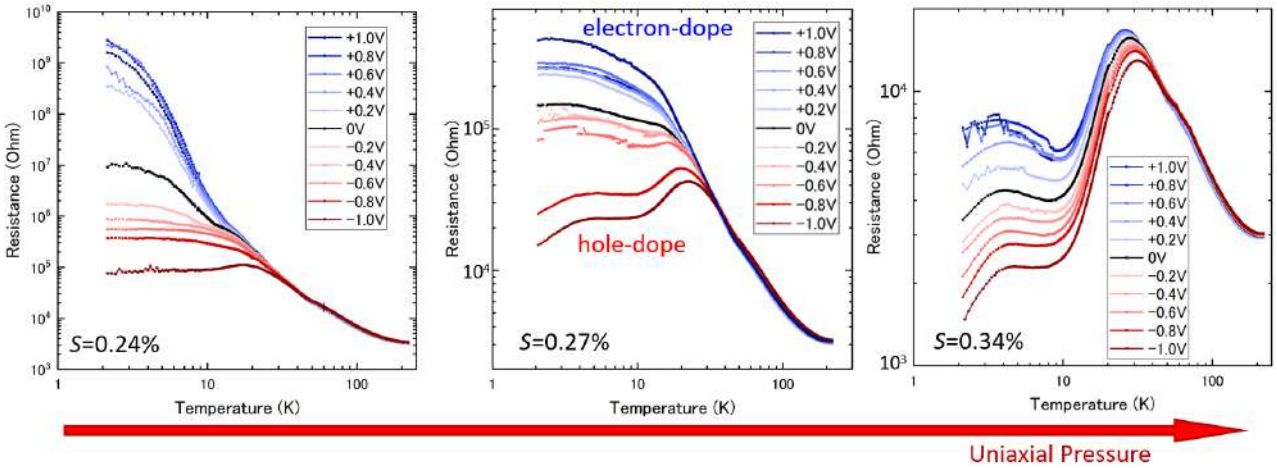

Fig. 2. Temperature dependence of the electric resistivity in the thin film of $EtMe_3P[Pd(dmit)_2]_2$ under the uniaxial pressure and carrier doping. *S* denotes the compression rate estimated from the curvature of the substrate.

This remains an open and interesting question.

For more systematic research, we are trying to apply uniaxial pressure along two different directions using a square-shaped soft substrate as shown in Fig. 3. The VBO phase of $EtMe_3P[Pd(dmit)_2]_2$ is associated with a triangular network of the antiferromagnetic 1/2-spins. Hence the effect of the uniaxial pressure on the thin-film crystal should be different from that of the hydrostatic pressure on the bulk crystal and the direction of the uniaxial pressure would affect physical properties. We aim to obtain a unified picture of the strongly correlated electron system by using our method for the simultaneous control of uniaxial pressure (band width) and carrier doping (band filling).

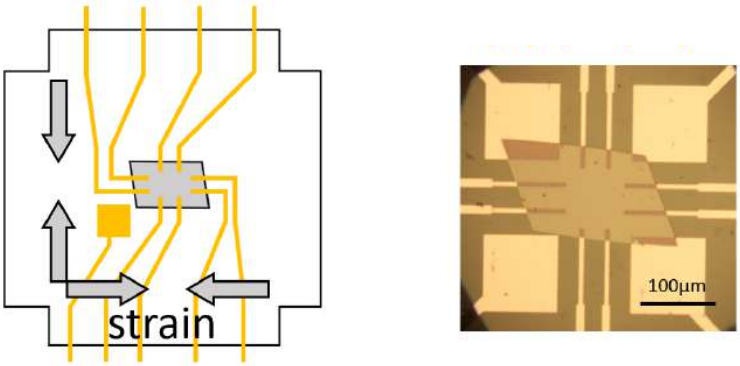

Fig. 3. Substrate and laminated thin crystal used in the method for uniaxial pressure along two directions.

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意義と波及効果：電子間相互作用が強い物質（強相関物質）はわずかなパラメータ変化によって多彩な電子状態を見せる。それらは物性物理研究の主要な対象物質のひとつであると同時に、電子相転移を利用した次世代デバイスへの応用が期待される。本研究では、重要なパラメータであるバンド占有率（ドーピング）とバンド幅（圧力）を同時に制御する新たな実験手法を分子性の強相関物質に適用する一環として、従来とは異なる基底状態を有する強相関物質を対象とし、その効果を確認した。このヘテロ界面を利用した電子状態制御法の適用範囲を今後さらに拡げることによって、強相関電子系の統一的な描像を得ることが期待できる。

Reference Data

Meson Science Laboratory
岩崎中間子科学研究室

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Masahiko IWASAKI Chief Scientist RIKEN Cluster for Pioneering Research Meson Science Laboratory 2-1 Hirosawa Wako Saitama 351-0198 JAPAN +81-(0) 48-467-9352 masa@riken.jp 
Education	1982-1987 Graduate School of Science, The University of Tokyo 1980-1982 The University of Tokyo, Faculty of Science, Department of Physics, 1977-1980 The University of Tokyo, College of General Education
Degrees	Dr. Sci. (1987) The University of Tokyo M. Sci. (1984) The University of Tokyo B. Sci. (1982) The University of Tokyo
Employment/research experience	2002- Chief Scientist, Meson Science Laboratory, RIKEN 1997-2002 Associate Professor, Graduate School of Science and Engineer-ing, Tokyo Institute of Technology 1987-1996 Assistant Professor, Meson Science Laboratory, Faculty of Sci-ence, University of Tokyo <u>Additional post</u> 2002-2020 Visiting Professor, Tokyo Institute of Technology 2011- Visiting Professor, KEK, The High Energy Accelerator Research Organization, Japan
	Riken BAIHO Award, RIKEN (2019) Inoue Prize for Science, Inoue Foundation for Promotion of Science (2005) Young Scientist Award for Experimental Nuclear Physics, Nuclear Science Forum (1994)
Academic activities	Member; Physical Society of Japan Member; Nuclear Physics Committee of Japan (2006-2018) Chair; Nuclear Physics Young Scientist Award Selection Panel (2016-) Member; Japan Meson Science Society Member; Organizing Committee of International Symposium on Exotic Atoms and Nuclei (1994-)

(1) Participants

Masahiko Iwasaki（岩崎 雅彦）	主任研究員
Katsuhiko Ishida（石田 勝彦）	協力研究員
Haruhiko Outa（應田 治彦）	専任研究員
Isao Watanabe（渡邊 功雄）	専任研究員
Kenta Itahashi（板橋 健太）	専任研究員
Fuminori Sakuma（佐久間 史典）	専任研究員
Yue Ma（馬　越）	専任研究員
Takumi Yamaga （山我 拓巳）	特別研究員
Hidemitsu Asano （浅野 秀光）	特別研究員
Rie Murayama (村山　理恵)	特別研究員
Sohtaro Kanda （神田 聡太郎）	基礎科学特別研究員
Retno Asih	JRA
Fahmi Astuti	JRA
Shintaro Tanaka（田中　慎太郎）	JRA
Shuu Aikawa（相川　脩）	JRA
Julia Angel	JRA
Muhamad Darwis	JRA
Masaya Ichikawa（市川　真也）	JRA
Toya Tanaka（田中　陶冶）	JRA
Shota Matsumoto（松本　翔汰）	JRA
Yoon Sungwon	IPA
Muhammad Redo Ramadhan	IPA
Harison Binti Rozak	IPA
Winarsih Suci	IPA
HAN Chengdong	IPA
Utami Widyaiswari	IPA
Muhammad Hanif Bin Che Lah	IPA
Irwan Ramli	研修生
Kazuhiro Tanaka（田中　万博）	客員主管研究員　(高エネルギー加速器研究機構)
Philip King	RAL 支所長（ISIS / RAL 支所）
Toshimitsu Yamazaki（山崎　敏光）	客員研究員（東京大学）
Eiichi Yagi（八木　栄一）	研究嘱託 （中間子科学研究室)
Zyun Ezawa（江澤　潤一）	客員研究員（東北大学)
Hiroyuki Noumi（野海　博之）	客員研究員（大阪大学核物理研究センター）
Shinji Okada（岡田　信二）	協力研究員（東原子分子物理研究室）
Tadashi Hashimoto（橋本　直 ）	客員研究員（日本原子力研究開発機構)
Takayasu Sekihara（関原　隆泰）	客員研究員（京都府立大学）
Dita Puspita Sari	客員研究員（芝浦工業大学）

(2) Original papers

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22. S. Ajimura et al.: "K^-pp", a Kbar-meson nuclear bound state, observed in $^3He(K^-, \Lambda p)n$ reactions, Physics Letters B **789**, 620-625 (2019) [1]
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24. B. V. Hampshire, K. Butcher, K. Ishida, G. Green, D. Paul and A. Hillier: "Using negative muons as a probe for depth profiling silver Roman coinage", Heritage 2019, **2**, 400-407 [2]
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27. M. A. Baqiya, T. Adachi, A. Takahashi, T. Konno, T. Ohgi, I. Watanabe, and Y. Koike: "Muon-spin Relaxation Study of the Spin Correlations in the Overdoped Regime of Electron-doped High-T_C Cuprate Superconductors" Phys. Rev. B **100**, 064514/1-5 (2019). [1]
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30. T. Takahashi, F. Sakuma, H. Ohnishi: "Hadron Physics at J-PARC", Prog. Part. Nucl. Phys., in press [1]

(3) Reviews and books（ Research Category in [ ] ）

1. 岩崎雅彦、野海博之:"クォークと反クォークが共存する原子核：K 中間子原子核の世界"，パリティ、2019 年 1 月号（Vol2019,No01） 第 34 巻第 1 号 p44-45 [1]
2. 岩崎雅彦、佐久間史典、山我拓巳:"最近の研究から：K 中間子と陽子 2 つからなる"奇妙な"原子核"、日本物理学会誌、2020 年 1 月号 第 75 巻第 1 号（通巻 855 号）p10-15. [1]

(4) Invited presentations（ Research Category in [ ] ）

1. 神田聡太郎: "Direct Measurement of Muonium Hyperfine Splitting; Apparatus Development and First Spectroscopy Result", 量子ビームサイエンスフェスタ、つくば, 2017 年 3 月. [2]
2. 石田勝彦: "ミューオン水素分光"、核物理の将来基礎物理班勉強会、茨城県東海村、2017 年 4 月. [2]
3. K. Ishida: "MuP HFS measurement with spin polarization", FAMU Meeting, Trieste, Italy, May 2017. [2]
4. K. Ishida: "Muon Facility at RIKEN-RAL", International Workshop on Organic Molecule Systems, Penang, Malaysia, August 2017. [2]
5. 神田聡太郎: "Precision laser spectroscopy of the muonic hydrogen HFS for determination of the proton radius", RCNP 研究会中性子と原子で探る基礎物理学, 吹田市、2017 年 8 月. [2]
6. 石田勝彦: "ミュオン水素原子の超微細構造エネルギー測定による陽子 Zemach 半径決定"、電子光理学研究センターセミナー、仙台、2017 年 8 月. [2]
7. S. Kanda: "Precision laser spectroscopy of the ground state hyperfine splitting in muonic hydrogen", NUFACT2017, Uppsala, Sweden, September 2017. [2]
8. K. Ishida: "Muon g-2/EDM at J-PARC", NUFACT2017, Uppsala, Sweden, September 2017. [2]
9. T. Hashimoto: "Kaonic nuclei studied via K- induced reactions at J-PARC", International Conference on Exotic Atoms and Related Topics (EXA2017), Vienna, 10-15 September 2017. [1]
10. M. Iwasaki: "Search for the simplest kaonic bound state K^-pp via $^3He(K^-,n)$ reaction at J-PARC", XVII International Conference on Hadron Spectroscopy and Structure (HADRON2017), Salamanca, Spain, 25-29 September 2017. [1]
11. M. Iwasaki: "Search for Kaonic Bound States at JPARC", 3rd Resonance Workshop in Bergamo, Camera di Commercio, Bergamo, Italy, 10-13 October 2017. [1]
12. F. Sakuma: "KbarNN bound state search at J-PARC E15", ASTRA: Advances and open problems in low-energy nuclear and hadronic STRAngeness physics, ECT*, Trento, Italy, 23-27 October 2017. [1]

13. K. Ishida: “Nuclear physics experiments using muons”, CSNS Seminar, Dongguan, China, December 2017. [2]
14. 石田勝彦: “理研 RAL ミュオン施設”、第 8 回 Muon 科学と加速器研究、つくば市、2018 年 1 月. [2]
15. 神田聡太郎: “Laser spectroscopy of the hyperfine splitting in the ground state of muonic hydrogen atom”、第 8 回 Muon 科学と加速器研究、つくば市、2018 年 1 月. [2]
16. 神田聡太郎: “Precision Laser Spectroscopy of the Ground State Hyperfine Splitting in Muonic Hydrogen”, 第 10 回 FPUA: Fundamental Physics Using Atoms, 名古屋, 2018 年 1 月. [2]
17. 神田聡太郎:, “超伝導計測のミューオン実験への応用”, TIA かけはし研究会, 和光, 2018 年 1 月. [2]
18. Sohtaro Kanda: “Precision Spectroscopy of Muonic Systems with High-intensity Pulsed Muon Beam”, Workshop on Lepton Flavor Physics with Most Intense DC Muon Beams, Tokyo, April 2018. [2]
19. F. Sakuma: “Search for the Kaonic Bound State KbarNN at J-PARC”, 15th International Workshop on Meson Physics (MESON2018), Krakow, Poland, 7-12 June 2018. [1]
20. F. Sakuma: “Search for the Kaonic Bound State KbarNN via ^{3}He(K^-, Λp/pΣπ)n Reactions”, YKIS2018b Symposium “Recent Developments in Quark-Hadron Sciences”, Yukawa Institute for Theoretical Physics, Kyoto University, 11-15 June, 2018. [1]
21. M. Iwasaki: “A quest for the "Kpp" bound state via 3He(K-,n) reaction, J-PARC E15 experiment”, The 13th International Conference on Hypernuclear and Strange Particle Physics (HYP2018), Portsmouth, VA23704, USA, 24-29 June 2018. [1]
22. Sohtaro Kanda: “Laser spectroscopy of the hyperfine splitting in muonic hydrogen atom by a measurement of decay electron asymmetry”, Nucleon Spin Structure at Low Q: A Hyperfine View, Trento, July 2018. [2]
23. 石田勝彦: “ミュオン原子による陽子半径決定”、大阪大学理学部物理セミナー、豊中、2018 年 8 月. [2]
24. Sohtaro Kanda: “Precision Spectroscopy of Exotic Atoms Involving Muon”, NuFact2018, Virginia, USA, August 2018. [2]
25. Sohtaro Kanda: “Laser spectroscopy of the ground-state hyperfine splitting in muonic hydrogen atom”, Symposium for Muon and Neutrino Physics 2018, Osaka, September 2018. [1]
26. 佐久間史典: “New Results on the "K^-pp" bound state from J-PARC”, 原子核中におけるハドロンの性質とカイラル対称性の役割, 東北大学電子光理学研究センター, 2018 年 9 月 11 日-12 日. [1]
27. I. Watanabe: “What is the muon spin relaxation (μSR) technique — How we can use that for the material science —“ The 19th International Conference in Asia (IUMRS-ICA 2018), Bali, Indonesia, 31 Oct-2 Nov 2018. [1]
28. K. Ishida: “Proton Zemach radius measurement by the hyperfine splitting of muonic hydrogen”, Fifth Joint Meeting of the Nuclear Physics Divisions of the American Physical Society and the Physical Society of Japan, Hawaii, USA, October 2018. [2]
29. T. Yamaga: “Results of KbarNN search via the (K^-, n) reaction at J-PARC”, The 8th International Conference on Quarks and Nuclear Physics (QNP2018), Tsukuba, Japan, 13-17 November 2018. [1]
30. F. Sakuma: “Kbar-Nuclear Bound State at J-PARC”, 13th International Conference on Nucleus-Nucleus Collisions (NN2018), Omiya, Saitama, Japan, 4-8 December 2018. [1]
31. Sohtaro Kanda: “Residual polarization and hyperfine transition rate in muonic hydrogen”, 新学術領域研究「宇宙観測検出器と量子ビームの出会い。新たな応用への架け橋。」キックオフシンポジウム, 仙台, 2018 年 12 月. [2]
32. K. Ishida: “Proton radius measurement with muonic atoms”, International workshop on the structure of the proton, Sagae, Yamagata, February 2019. [2]
33. Sohtaro Kanda: “Development of instruments for the proton radius measurement at RIKEN”, International workshop on the structure of the proton, Sagae, Yamagata, February 2019. [2]
34. 石田勝彦: “ミュオン原子による陽子 Zemach 半径測定”、電子光理学研究センター拠点研究会「電子散乱による原子核研究ー陽子半径、不安定核の電荷密度分布を中心にー」、東北大学電子光理学研究センター、仙台、2019 年 3 月. [2]
35. F. Sakuma: “K-pp bound system at J-PARC”, The 15th International Conference on Meson-Nucleon Physics and the Structure of the Nucleon (MENU-2019), Cohon University Center, Carnegie Mellon

University, Pittsburgh Pennsylvania, 2-7 June 2019. [1]

36. K. Ishida: “Status of the g-2 and EDM experiment at J-PARC”, FCCP2019, Anacapri, Italy, August 2019. [2]
37. K. Ishida: “Measurement of the proton Zemach radius from the hyperfine splitting in muonic hydrogen utilizing muon spin repolarization with laser: Principle and Method”, Proton Radius 2019, Veli Losinji, Croatia, September 2019. [2]
38. S. Kanda: “Measurement of the proton Zemach radius from the hyperfine splitting in muonic hydrogen utilizing muon spin repolarization with laser: Preparation Status”, Proton Radius 2019, Veli Losinji, Croatia, September 2019. [2]
39. K. Ishida: “Status of the g-2 and EDM experiment at J-PARC”, Proton Radius 2019, Veli Losinji, Croatia, September 2019. [2]
40. M. Iwasaki: “Kaonic Nuclear Bound State "K^-pp" Observation and Possible Future Plan”、The 3rd J-PARC symposium (J-PARC2019), Tsukuba, Japan, 23-26 September 2019. [1]
41. K. Ishida et al.: “Laser spectroscopy of the 1s hyperfine splitting energy of muonic hydrogen for the determination of proton Zemach radius”, The 3rd J-PARC symposium (J-PARC2019), Tsukuba, Japan, 23-26 September 2019. [2]
42. I. Watanabe: “Advanced Material Science Activity in Japan under Collaborations with Indonesian Groups” The 1st International MIPAnet Conference on Science and Mathematics (IMC-SciMath 2019), Parapat, Indonesia, 9-11 October 2019. [1]
43. M. Iwasaki: “A novel and peculiar quantum system - K-meson and two protons bound state”, STRANEX: Recent progress and perspectives in STRANge EXotic atoms studies and related topics ECT*, Trento, 21-25 October 2019. [1]
44. F.Sakuma: “Λ(1405)pn Final State in the K^- + ^{3}He reaction”, STRANEX: Recent progress and perspectives in STRANge EXotic atoms studies and related topics ECT*, Trento, 21-25 October 2019. [1]
45. I. Watanabe: “Multi-Angle Approach to Magnetic Properties of Nano-State $La_{2-x}Sr_xCuO_4$” 4th Padjadjaran International Physics Symposium (PIPS2019), Bandung, Indonesia, 13-14 November 2019. [1]
46. I. Watanabe: “How We can Approach to Magnetic Properties of Nano-State $La_{2-x}Sr_xO_4$” International Conference on Magnetism and Its Application (ICMIA2019), Solo, Indonesia, 20-21 November 2019. [1]
47. 石田勝彦: “英国理研 RAL ミュオン施設とミュオン利用分析”、第 2 回文理融合シンポジウム 量子ビームで歴史を探る —加速器が紡ぐ文理融合の地平—、大阪市、2019 年 12 月. [2]

(5) Patent applications（ Research Category in [ ] ）

N/A

(6) Collaborations including both inside and outside project（ Research Category in [ ] ）

1. 岩崎雅彦、野海博之(阪大)、大西宏明(東北大)、永江知文(京大)、橋本直(JAEA)、Catalina Oana Curceanu(INFN(Italy))、Johann Zmeskal(SMI(Austria)) 、小沢恭一郎(KEK/東大) 、飯尾雅実(KEK/J-PARC)：J-PARC での K 中間子原子核実験 [1]
2. 野海博之(阪大)、岩崎雅彦：連続データ収集システム開発 [2]
3. 岩崎雅彦、東俊行、岡田信二、橋本直(JAEA)、超伝導転移点検出器 TES 応用研究[2]
4. 岩崎雅彦、石田勝彦、渡邊功雄、Philip King、Adrian Hillier（RAL/STFC）：理研 RAL ミュオン施設での μSR・ミュオン原子研究[1,2,3]
5. 岩崎雅彦、石田勝彦、神田聡太郎、和田智之、斉藤徳人、湯本正樹（光量子工学研究センター）：ミュオン水素原子励起用中赤外レーザー開発 [2]
6. 渡邊功雄、後藤孝行、足立匡、黒江晴彦（上智大）：ナノサイズ酸化物高温超伝導体の磁性と超伝導の研究 [1]
7. 渡邊功雄、石井康之、Dita Puspita Sari(芝浦工業大学)：有機超伝導体の μSR 研究 [1]
8. 渡邊功雄、幸田章宏（KEK/J-PARC）：強相関電子系物質の μSR 研究 [1]

9. 渡邊功雄、小池洋二、川股隆行（東北大学）：銅酸化物高温超電導体の μSR 研究 [1]
10. 渡邊功雄、河本充司、福岡脩平（北海道大学）：有機磁性体、有機超伝導体の μR 研究 [1]
11. 渡邊功雄、市村晃一（北海道大学）：DNA の STM 研究 [1]
12. 渡邊功雄、小形正男、松浦弘康、檜原太一（東京大学）：ミュオン位置計算手法開発 [1]
13. 渡邊功雄、谷口浩三、小林拓矢（埼玉大）：有機分子性磁性体の NMR・μSR 研究 [1]

(7) Hosted seminars and symposiums

1. RIKEN Symposium "International Workshop on Organic Molecule Systems", Penang, Malaysia, 1-3 August 2017.
2. RIKEN Symposium "3rd Emallia Conference 2017", Busan, Korea, 7-8 September 2017.
3. RIKEN Symposium "4th Emallia Conference 2018", Sapporo, Hokkaido 23-24 July 2018.
4. RIKEN Symposium "The 4th International Conference on Functional Materials Science 2018", Bali, Indonesia, 14-15 November 2018.
5. RIKEN Symposium "International Workshop of Topological Quantum Materials", Tainan, Taiwan, 10-12 January 2019.
6. RIKEN Symposium "The 5th International Symposium in Current Progress in Mathematics and Sciences", Depok, Indonesia, 9-10 July 2019.
7. 第 10 回「Muon 科学と加速器研究」、理研、和光市、2020 年 1 月 8-9 日.

(8) Awards and honors

1. F. Astuti: International Workshop on Organic Molecule Systems, Batu Feringgih, Malaysia 2017, Poster Prize
2. D.P. Sari: International Workshop on Organic Molecule Systems, Batu Feringgih, Malaysia 2017, Poster Prize
3. R. Ramadhan: RIKEN Summer School 2017, Poster Prize (in Physics）
4. S. Winarsih: The 4th International Conference on Functional Materials Science 2018, Bali, Indonesia, Poster Prize
5. J. Angel: The 4th International Conference on Functional Materials Science 2018, Bali, Indonesia, Poster Prize
6. M. Iwasaki: Riken BAIHO Award, RIKEN (2019)
7. S. Winarsih: RIKEN Summer School 2019, Poster Prize（in Physics）
8. S. Winarsih: RIKEN Summer School 2019, Poster Prize（Best Presentation）
9. S. Winarsih: RIKEN Exchange Meeting, Poster Prize（Student Section）

(9) Press releases

1. "Worldwide first observation of the two-dimensional ferromagnetic fluctuation in the Cu-based high-temperature superconducting oxides –Elucidation of the whole view of magnetic states in high-temperature superconducting oxides—", Sophia University, RIKEN, Tohoku University, Institute for Materials Research (IMR), KEK, J-PARC Center, Aug. 2018
   2018 年 8 月 3 日「銅酸化物高温超伝導体で 2 次元の強磁性揺らぎを世界で初めて観測 −高温用伝導体の磁性状態の全貌を解明−」上智大学・理化学研究所・東北大学・金属材料研究所・高エネルギー加速器研究機構・J-PARC センター
   https://www.riken.jp/press/2018/20180803_3/index.html
2. "Scientists observe a new form of strange matter", RIKEN, KEK, JAEA, U. Osaka, Istituto Nazionale di Fisica Nucleare (INFN), The Stefan Meyer Institute (SMI), J-PARC, Jan. 2019, [1]
   「K-中間子と二つの陽子からなる原子核の発見 -クォークと反クォークが共存する"奇妙な"結合状態-」, 理化学研究所、高エネルギー加速器研究機構、日本原子力研究開発機構、大阪大学、東北大学、INFN、SMI、J-PARC センター, 2019 年 1 月 24 日
   https://www.riken.jp/press/2019/20190124_2/index.html

Nuclear Spectroscopy Laboratory
上野核分光研究室

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Hideki UENO Chief Scientist / Group Director RIKEN Cluster for Pioneering Research & RIKEN Nishina Center for Accelerator-Based Science Nuclear Spectroscopy Laboratory 2-1 Hirosawa Wako Saitama 351-0198 JAPAN +81-(0)48-462-7681 (ext. 4813) ueno@riken.jp 
Education	1991−1995 Graduate School of Science and Engineering, Tokyo Institute of Technology 1987−1991 Department of Applied Physics, Faculty of Science, Tokyo Institute of Technology
Degrees	Dr. Sci. (1996) Tokyo Institute of Technology M. Sci. (1993) Tokyo Institute of Technology B. Sci. (1991) Tokyo Institute of Technology
Employment/research experience	2018− Group Director, User Liaison Group, RIKEN Nishina Center for Accelerator-Based Science (RNC) 2018− Team Leader, Outreach Team, RNC 2016−2018 Group Director, Research Instruments Group, RNC 2013− Chief Scientist, Nuclear Spectroscopy Laboratory, RIKEN (main duty) 2010−2016 Deputy Group Director, User Liaison and Industrial Cooperation Group, RNC 2010−2013 Team Leader, RIBF User Liaison Team, RNC 2009−2013 Team Leader, Polarized RI Beam Team, RNC 2005−2009 Senior Research Scientist, Applied Nuclear Physics Laboratory, RIKEN (Internal transfer to Polarized RI Beam Team, RNC, 2007−2009) 2000−2005 Research Scientist, Applied Nuclear Physics Laboratory, RIKEN 1995−2000 Research Associate, Laboratory of Nuclear Studies, Osaka University 1995 Research Fellow of the Japan Society for the Promotion of Science <u>Additional post</u> 2015− Visiting Professor, Meiji University 2015−2018 Visiting Professor, Osaka University 2011−2016 Visiting Professor, Tokyo Institute of Technology 2011− Visiting Professor, Rikkyo University 2009−2011 Visiting Associate Professor, Tokyo Institute of Technology 2006−2011 Visiting Associate Professor, Rikkyo University
Awards and honors	JPS Award for Academic Papers on Physics (2013) Young Scientist Prize of Japan Nuclear Experiment Physics Forum (1997)

Academic activities	Member; The Physical Society of Japan (1992−present) Member; International Advisory Committee of the Hyperfine Interactions conference series (2019−present) Member; Shared-use Steering Committee of Heavy Ion Medial Accelerator in Chiba (HIMAC), National Institutes for Quantum and Radiological Science and Technology (QST) (2018−present) Member; Program Advisory Committee for the Laser Electron Photon Experiment at SPring-8 (LEPS), RCNP, Osaka University (2014−2018) Member; Physics Program Advisory Committee for RCNP, Osaka University (2014−2016) Member; Program Committee of the Joint Meeting of the Nuclear Physics Divisions of the American Physical Society and The Physical Society of Japan (2014, 2020−present) Member; Scientific Secretary of JPS Division of Experimental Nuclear Physics (2013−2014) Member; International Advisory Board of "Prague meetings on Spin Research Programme Advanced Studies Institute − Symmetries and Spin" (2008−2013) Member; Program Advisory Committee for Nuclear-Physics Experiments at RIKEN Accelerator Research Facility (2003−2006)

(1) Participants

Hideki Ueno（上野 秀樹）	主任研究員／室長
Hiroki Yamazaki（山崎 展樹）	専任研究員
Yuichi Ichikawa（市川 雄一）	専任研究員
Aiko Takamine（高峰 愛子）	研究員
Minori Tajima（田島 美典）	特別研究員
Kei Imamura（今村 慧）	特別研究員
Aleksey Gladkov	リサーチアソシエイト
Tomoya Sato（佐藤 智哉）	基礎科学特別研究員
Keita Kawata（川田 敬太）	JRA（東京大学)
Yukari Matsuo（松尾 由賀利）	客員主管研究員（法政大学)
Jean-Michel Daugas	客員研究員（CEA）
Georgi Georgiev	客員研究員（CNRS/IN2P3/CSNSM)
Deyan T. Yordanov	客員研究員（CNRS/IN2P3/IPN Orsay)
Dimiter L. Balabanski	客員研究員（IFIN-HH）
Xiaofei Yang	客員研究員（KU Leuven）
Andrew E. Stuchbery	客員研究員（The Australian National University)
Akihiro Yoshimi（吉見 彰洋）	客員研究員（岡山大学)
Hiroki Nishibata（西畑 洸希）	客員研究員（九州大学)
Yoko Ishibashi（石橋 陽子）	客員研究員（東北大学）
Yoshio Kobayashi（小林 義男）	客員研究員（電気通信大学)
Timothy J. Gray	研修生（The Australian National University)
Aiko Uchiyama（内山 愛子）	研修生（東北大）
Yutaro Nakamura（中村 祐太郎）	研修生（明治大学）
Fumiya Yokosuka（横須賀 文哉）	研修生（青山学院大学)
Takashi Kawaguchi（川口 高史）	研修生（法政大学)
Makoto Sanjo（三條 真）	研修生（法政大学)
Wataru Kobayashi（小林 航）	研修生（法政大学)
Yusuke Sasaki（佐々木 悠輔）	研修生（法政大学)
Takumi Asakawa（浅河 拓光）	研修生（法政大学)
Yuika Takeuchi（竹内 由衣花）	研修生（法政大学)
Taichi Akaoka（赤岡 太一）	研修生（法政大学)
Airi Toda（戸田 愛梨）	研修生（法政大学)
Takumi Yamamoto（山本 匠）	研修生（法政大学)
Masaki Nishimura（西村 昌輝）	研修生（法政大学)
Miru Doi（土居 三瑠）	研修生（法政大学)
Kenta Tsubura（螺良 健太）	研修生（法政大学)

(2) Original papers（Research Category in [ ]）

1. H. Nishibata, T. Shiomoda, A. Odahara, S. Morimoto, S. Kanaya, A. Yagi, H. Kanaoka, M. R. Pearson, C. D. P. Levy, M. Kimura, "Shape coexistence in the $N = 19$ neutron-rich nucleus ^{31}Mg explored by β-γ spectroscopy of spin-polarized ^{31}Na," Phys. Lett. B **767**, 81–85 (2017). [2]
2. N. Yamanaka, B. K. Saoo, N. Yoshinaga, T. Sato, K. Asahi, B. P. Das, "Probing exotic phenomena at the interface of nuclear and particle physics with the electric dipole moments of diamagnetic atoms: A unique window of hadronic and semi-leptonic CP violation," Eur. Phys. J. A **53**, 54 (2017). [1]
3. M. Hase, Y. Ebukuro, H. Kuroe, M. Matsumoto, A. Matsuo, K. Kindo, J. R. Hester, T. J. Sato, H. Yamazaki, "Magnetism of the antiferromagnetic spin-3/2 dimer compound $CrVMoO_7$ having an antiferromagnetically ordered state," Phys. Rev. B **95**, 144429 (2017). [3]
4. R. Miyatani, Y. Kobayashi, Y. Yamada, "Thermal reaction of sonochemically prepared amorphous Fe/C," Hyperfine Interact. **238**, 61-1–8 (2017). [3]

5. N. Nishida, S. Amagasa, Y. Kobayashi, Y. Yamada, "Mixture of silver and iron oxide nanoparticles produced by chemical methods," Hyperfine Interact. **238**, 71-1–7 (2017). [3]
6. H. Ito, S. Amagasa, N. Nishida, Y. Kobayashi, Y. Yamada, "Wet chemical synthesis of zinc-iron oxide nanocomposite," Hyperfine Interact. **238**, 79-1–9 (2017). [3]
7. S. Amagasa, N. Nishida, Y. Kobayashi, Y. Yamada, "Effect of laser irradiation on iron carbide nanoparticles produced by laser ablation in ethanol," Hyperfine Interact. **238**, 83-1–8 (2017).
8. I. Kubono, N. Nishida, Y. Kobayashi, Y. Yamada, "Mössbauer spectra of iron (III) sulfide particles," Hyperfine Interact. **238**, 91-1–10 (2017). [3]
9. M. Mukai, Y. Hirayama, Y. X. Watanabe, P. Schury, H. S. Jung, M. Ahmed, H. Haba, H. Ishiyama, S. C. Jeong, Y. Kakiguchi, S. Kimura, J.Y. Moon, M. Oyaizu, A. Ozawa, J. H. Park, H. Ueno, M. Wada, H. Miyatake, "High-efficiency and low-background multi-segmented proportional gas counter for β-decay spectroscopy," Nucl. Instrum. Methods Phys. Res. A **884**, 1–10 (2018). [1, 2]
10. T. Sato, Y. Ichikawa, S. Kojima, C. Funayama, S. Tanaka, T. Inoue, A. Uchiyama, A. Gladkov, A. Takamine, Y. Sakamoto, Y. Ohtomo, C. Hirao, M. Chikamori, E. Hikota, T. Suzuki, M. Tsuchiya, T. Furukawa, A.Yoshimi, C. P. Bidinosti, T. Ino, H. Ueno, Y. Matsuo, T. Fukuyawa, N. Yoshinaga, Y. Sakemi, K. Asahi, "Development of co-located ^{129}Xe and ^{131}Xe nuclear spin masers with external feedback scheme," Phys. Lett. A **382**, 588 (2018). [1]
11. Y. Ito, P. Schury, M. Wada, F. Arai, H. Haba, Y. Hirayama, S. Ishizawa, D. Kaji, S. Kimura, H. Koura, M. MacCormick, H. Miyatake, J. Y. Moon, K. Morimoto, K. Morita, M. Mukai, I. Murray, T. Niwase, K. Okada, A. Ozawa, M. Rosenbusch, A. Takamine, T. Tanaka, Y. X. Watanabe, H. Wollnik, and S. Yamaki, "First mass measurements of nuclides around $Z = 100$ with a multireflection time-of-flight mass spectrograph," Phys. Rev. Lett. **120**, 152501 (2018). [1]
12. O. B. Tarasov, D. S. Ahn, D. Bazin, N. Fukuda, A. Gade, M. Hausmann, N. Inabe, S. Ishikawa, N. Iwasa, K. Kawata, T. Komatsubara, T. Kubo, K. Kusaka, D. J. Morrissey, M. Ohtake, H. Otsu, M. Portillo, T. Sakakibara, H. Sakurai, H. Sato, B. M. Sherrill, Y. Shimizu, A. Stolz, T. Sumikama, H. Suzuki, H. Takeda, M. Thoennessen, H. Ueno, Y. Yanagisawa, and K. Yoshida, "Discovery of ^{60}Ca and implifications for the stability of ^{70}Ca," Phys. Rev. Lett. **121**, 022501 (2018). [1]
13. M. Hase, Y. Ebukuro, H. Kuroe, M. Matsumoto, A. Matsuo, K. Kindo, J. R. Hester, T. J. Sato, and H. Yamazaki, "Erratum: Magnetism of the antiferromagnetic spin-32 dimer compound $CrVMoO_7$ having an antiferromagnetically ordered state [Phys. Rev. B **95**, 144429 (2017)]," Phys. Rev. B **98**, 139901 (2018). [1]
14. B. A. Marsh, T. Day Goodacre, S. Sels, Y. Tsunoda, B. Andel, A. N. Andreyev, N. A. Althubiti, D. Atanasov, A. E. Barzakh, J. Billowes, K. Blaum, T. E. Cocolios, J. G. Cubiss, J. Dobaczewski, G. J. Farooq-Smith, D. V. Fedorov, V. N. Fedosseev, K. T. Flanagan, L. P. Gaffney, L. Ghys, M. Huyse, S. Kreim, D. Lunney, K. M. Lynch, V. Manea, Y. Martinez Palenzuela, P. L. Molkanov, T. Otsuka, A. Pastore, M. Rosenbusch, R. E. Rossel, S. Rothe, L. Schweikhard, M. D. Seliverstov, P. Spagnoletti, C. Van Beveren, P. Van Duppen, M. Veinhard, E. Verstraelen, A. Welker, K. Wendt, F. Wienholtz, R. N. Wolf, A. Zadvornaya, K. Zuber, "Characterization of shape-staggering effect in mercury nuclei," Nat. Phys. **14**, 1163 (2018). [1]
15. S. Kimura, Y. Ito, D. Kaji, P. Schury, M. Wada, H. Haba, T. Hashimoto, Y. Hirayama, M. MacCormick, H. Miyatake, J. Y. Moon, K. Morimoto, M. Mukai, I. Murray, A. Ozawa, M. Rosenbusch, H. Schatz, A. Takamine, T. Tanaka, Y. X. Watanabe, H. Wollnik, "Atomic masses of intermediate-mass neutron-deficient nuclei with relative uncertainty down to 35-ppb via multireflection time-of-flight mass spectrograph," Int. J. Mass Spectrom. **430**, 134 (2018). [1]
16. Z. Y. Xu, H. Heylen, K. Asahi, F. Boulay, J. M. Daugas, R. P. de Groote, W. Gins, O. Kamalou, Á. Koszorús, M. Lykiardopoulou, T. J. Mertzimekis, G. Neyens, H. Nishibata, T. Otsuka, R. Orset, A. Poves, T. Sato, C. Stodel, J .C. Thomas, N. Tsunoda, Y. Utsuno, M. Vandebrouck, X. F. Yang, "Nuclear moments of the low-lying isomeric 1^+ state of ^{34}Al: Investigation on the neutron 1p1h excitation across $N = 20$ in the island of inversion," Phys. Lett. B **782**, 619–626 (2018). [2]
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19. N. Nishida, S. Amagasa, H. Ito, Y. Kobayashi, Y. Yamada, "Manganese-doped feroxyhyte nano-urchins produced by chemical methods," Hyperfine Interact. **239**, 33-1–8 (2018). [3]
20. K. Imamura, Y. Matsuo, W. Kobayashi, T. Egami, M. Sanjo, A. Takamine, T. Fujita, D. Tominaga, Y. Nakamura, T. Furukawa, T. Wakui, Y. Ichikawa, H. Nishibata, T. Sato, A. Gladkov, L. C. Tao, T. Kawaguchi, Y. Baba, M. Iijima, H. Gonda, Y. Takeuchi, R. Nakazato, H. Odashima, and H. Ueno, "Absolute optical absorption cross-section measurement of Rb atoms injected into superfluid helium using energetic ion beams," App. Phys. Exp. **12**, 016502 (2019). [3]
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23. H. Nishibata, S. Kanaya, T. Shimoda, A. Odahara, S. Morimoto, A. Yagi, H. Kanaoka, M. R. Pearson, C. D. P. Levy, M. Kimura, N. Tsunoda, and T. Otsuka, "Structure of ^{31}Mg: Shape coexistence revealed by β-γ spectroscopy with spin-polarized ^{31}Na," Phys. Rev. C **99**, 024322 (2019). [2]
24. M. Tajima, N. Kuroda, C. Amsler, H. Breuker, C. Evans, M. Fleck, A. Gligorova, H. Higaki, Y. Kanai, B. Kolbinger, A. Lanz, M. Leali, V. Mäckel, C. Malbrunot, V. Mascagna, Y. Matsuda, D. Murtagh, Y. Nagata, A. Nanda, B. Radics, M. Simon, S. Ulmer, L.Venturelli, E. Widmann, M. Wiesingerc, Y. Yamazaki, "Antiproton beams with low energy spread for antihydrogen production," J. Instrum. **14**, P05009 (2019). [1]
25. L. C. Tao, Y. Ichikawa, C. X. Yuan, Y. Ishibashi, A. Takamine, A. Gladkov, T. Fujita, K. Asahi, T. Egami, C. Funayama, K. Imamura, J. L. Lou, T. Kawaguchi, S. Kojima, T. Nishizaka, T. Sato, D. Tominaga, X. F. Yang, H. Yamazaki, Y. L. Ye, H. Ueno, Y. Yanagisawa, K. Yoshida, "Negative parity states in ^{39}Cl configured by crossing major shell orbits," Chin. Phys. Lett. **36**, 062101-1–4 (2019). [1, 2]
26. D. S. Ahn, N. Fukuda, H. Geissel, N. Inabe, N. Iwasa, T. Kubo, K. Kusaka, D. J. Morrissey, D. Murai, T. Nakamura, M. Ohtake, H. Otsu, H. Sato, B. M. Sherrill, Y. Shimizu, H. Suzuki, H. Takeda, O. B. Tarasov, H. Ueno, Y. Yanagisawa, K. Yoshida, "Location of the neutron dripline at fluorine and neon," Phys. Rev. Lett. **123**, 212501-1–6 (2019). [1]
27. T. Funabashi, Y. Kobayashi, Y. Yamada, "Metastable iron carbide thin films produced by pulsed laser deposition of iron in methane atmosphere," Hyperfine Interact. **240**, 121-1–8 (2019). [3]
28. F. Boulay, G. S. Simpson, Y. Ichikawa, S. Kisyov, D. Bucurescu, A. Takamine, D. S. Ahn, K. Asahi, H. Baba, D. L. Balabanski, T. Egami, T. Fujita, N. Fukuda, C. Funayama, T. Furukawa, G. Georgiev, A. Gladkov, M. Hass, K. Imamura, N. Inabe, Y. Ishibashi, T. Kawaguchi, T. Kawamura, W. Kim, Y. Kobayashi, S. Kojima, A. Kusoglu, R. Lozeva, S. Momiyama, I. Mukul, M. Niikura, H. Nishibata, T. Nishizaka, A. Odahara, Y. Ohtomo, D. Ralet, T. Sato, Y. Shimizu, T. Sumikama, H. Suzuki, H. Takeda, L. C. Tao, Y. Togano, D. Tominaga, H. Ueno, H. Yamazaki, X. F. Yang, J. M. Daugas, "*g*-Factor of the ^{99}Zr ($7/2^+$) isomer: Monopole evolution in shape coexisting region," Phys. Rev. Lett. **124**, 112501 (2020). [2]
29. K. Hamazaki, Y. Kobayashi, Y. Yamada, "Iron nitride films produced by arc deposition of iron in a nitrogen atmosphere," Hyperfine Interact. **241**, 4-1–10 (2020). [3]
30. Y. Yamada, Y. Sato, Y. Kobayashi, T. Ando, N. Takahama, K. Some, M. Sato, M. Mihara, M. K. Kubo, W. Sato, J. Miyazaki, T. Nagatomo, J. Kobayashi, A. Okazawa, S. Sato, A. Kitagawa, "In-beam

Mössbauer spectra for ^{57}Mn implanted sulfur hexafluoride," Hyperfine Interact. **241**, 15-1–15 (2020). [3]

(3) Reviews and books （ Research Category in [ ] ）

1. 市川雄一: "変形しながら殻進化—磁気モーメントで探るエキゾチック核の「中身」—" アイソトープニュース **765**, 26–29 (2019). [2]

(4) Invited presentations （ Research Category in [ ] ）

1. Y. Ichikawa: "Magnetic moment measurement of isomeric state of ^{75}Cu using spin-aligned RI beam at RIBF", Advances in Radioactive Isotope Science 2017 (ARIS 2017), Keystone, USA, May 28 – June 2 (2017). [2]
2. H. Ueno: "Nuclear moment and shell model", Ito International Research Center (IIRC) Symposium – Perspective of the physics of nuclear structure −, Tokyo, Japan, November 1−4 (2017). [1, 2]
3. Y. Ichikawa: "Nuclear moment measurement using spin-oriented RI beam at RIBF", International Symposium on RI Beam Physics in the 21st Century: 10th Anniversary of RIBF, Wako, Japan, December 4−5 (2017). [2]
4. H. Nishibata, T. Shimoda, A. Odahara, S. Morimoto, S. Kanaya, A. Yagi, H. Kanaoka, M. R. Pearson, C. D. P. Levy, M. Kimura: "Shape coexistence in ^{31}Mg revealed by β- and β-γ spectroscopy with spin-polarize ^{31}Na," The IX International Symposium on Exotic Nuclei (EXON2018), Petrozavodsk, Russia, September 1–15 (2018). [1, 2]
5. T. Sato: "Coexisting Xe-129 and Xe-131 masers with active feedback scheme for Xe atomic EDM search," Fifth Joint Meeting of the Nuclear Physics Divisions of the APS and the JPS (HAWAII2018), Waikoloa, Hawaii, USA, October 23–27 (2018). [1]
6. T. Sato: "Atomic EDM searches in RIKEN," The 10th China-Japan Joint Nuclear Physics Symposium (CJNP2018), Huizhou, China, November 18–23 (2018). [1]
7. H. Ueno: "R&D of spin-controlled RI beams," The 10th China-Japan Joint Nuclear Physics Symposium (CJNP2018), Huizhou, China, November 18–23 (2018). [1]
8. M. Tajima: "Laser spectroscopy of RI beams at the SLOWRI facility of RIKEN," The 10th China-Japan Joint Nuclear Physics Symposium (CJNP2018), Huizhou, China, November 18–23 (2018). [1]
9. Y. Ichikawa: "Nuclear magnetic dipole moments measured with spin-oriented RI beams at RIKEN RIBF," The International Conference on HYPERFINE Interactions and Applications (HYPERFINE 2019), Goa, India, February 10–15 (2019). [2]
10. A. Takamine, "Recent progress in the development of gas cells, SHE results combining GARIS with GASCELL+MRTOF," Expert Meeting on Next-Generation Fragment Separators 2019, Darmstadt, Germany, September 30–October 3 (2019). [1]
11. H. Ueno, "Nuclear-physics research based on RI spin orientation technique," XXXVI Mazurian Lakes Conference on Physics, Piaski, Poland September (2019). [1, 2, 3]
12. Y. Ichikawa, "Magnetic-moment measurement of exotic nuclei using spin-oriented RI beams at RIBF," 14th Asia-Pacific Physics Conference (APPC 2019), Sarawak, Malaysia, November 17–22 (2019). [2]

(5) Patent applications （ Research Category in [ ] ）

N/A

(6) Collaborations including both inside and outside project （ Research Category in [ ] ）

1. 市川 雄一、大塚 孝治（東京大学）、角田 佑介（東京大学）: 京コンピュータを用いた ^{75}Cu 核の大規模殻模型計算 [2]

2. 市川 雄一、清水 則孝（東京大学）、宇都野 穣（JAEA）：^{39}Cl 核の殻模型計算 [2, 1]
3. 大塚 孝治（東京大学）、角田 直文（東京大学）、清水 則孝（東京大学）、上野 秀樹：遠不安定原子核の束縛条件に関する理論的研究 [1]
4. 市川 雄一、吉田 賢一（京大）、加須屋 春樹（京大基研）：平均場理論を用いた奇質量核の核モーメント計算 [1, 2]
5. 市川雄一、D. Bucurescu（IFIN-HH）、S. Kisyov（IFIN-HH）: Interacting boson-fermion mode (IBFM) に基づくによる ^{99}Zr 核モーメントの計算 [2]
6. 旭 耕一郎、佐藤 智哉、市川 雄一、B.P. Das（東工大）：反磁性原子の原子 EDM（電気双極子モーメント）の理論計算 [1]
7. 旭 耕一郎、佐藤 智哉、市川 雄一、清水 則孝（東大 CNS）、吉永 尚孝（埼玉大）：大規模殻模型によるシッフモーメント計算 [1]
8. 上野秀樹、竹内由衣花、松尾由賀利（法政大学）、善甫康成（法政大学）：超流動ヘリウム中原子バブル半径の密度汎関数法計算 [3]
9. 上野秀樹、藤田朋美、松尾由賀利（法政大学）、善甫康成（法政大学）：超流動ヘリウム中原子の超微細構造間隔のファンデルワールス半径依存性 [3]
10. 山崎 展樹、西畑 洸希、藤山 茂樹（加藤分子物性研究室）：物質中の電場勾配計算 [3]
11. 山崎 展樹、渡邊 功雄（中間子科学研究室）：物質中電場勾配の第一原理計算 [3]
12. 山崎 展樹、山瀬 博之（物質・材料研究機構）：金属におけるバンド計算 [3]
13. 山崎 展樹、Balazs Ujfalussy（Hungarian Academy of Science）、James F. Annett（University of Bristol）: 相対論的スピン偏極 KKR 理論による Nb/Au/Fe３層膜における超伝導近接効果の計算 [3]
14. 山崎 展樹、Nic Shannon（OIST）：スピン軌道相互作用のある系における超伝導近接効果の理論的考察 [3]

(7) Hosted seminars and symposiums

1. 「Development of isomer beam by fragmentation reactions」、川太敬太氏（東大 CNS）、埼玉県和光市、2017 年 5 月 17 日（第 21 回核分光研セミナー）
2. 「The development of a low-background gas-counter and hyperfine structure measurement for neutron-rich iridium isotopes」、向井もも（筑波大）、埼玉県和光市、2017 年 5 月 17 日（第 22 回核分光研セミナー）
3. 第２回 ExpRes 道場 “Data Acquisition、” 2017 年 10 月 6 日
4. 「Ps- photodetachment spectroscopy and its application」、長嶋泰之（東京理科大）、埼玉県和光市、2017 年 10 月 18 日（第 23 回核分光研セミナー）
5. “Ito International Research Center (IIRC) Symposium: Perspectives of the physics of nuclear structure”, November 1−4（2017）.
6. 「高温超伝導銅酸化物の物質と物性 Cuprate high-T_c superconductors: Materials and Properties」、山本文子（芝浦工業大学）、埼玉県和光市、2018 年 1 月 26 日（第 24 回核分光研セミナー）
7. 理研新領域開拓課題「物質階層原理研究」&「ヘテロ界面研究」合同春期研究会、熱海市、2018 年 5 月 11−12 日.
8. 「Si/CdTe 半導体コンプトンカメラの開発研究と高感度 MeV ガンマ線観測実現に向けた展望」、渡辺伸 （宇宙航空研究開発機構（JAXA） 宇宙科学研究所（ISAS））、埼玉県和光市、2018 年 9 月 27 日（第 25 回核分光研 & 新学術領域研究「量子ビーム応用 」B03 合同セミナー）
9. 新学術領域研究「宇宙観測検出器と量子ビームの出会い。新たな応用への架け橋。」キックオフシンポジウム、仙台、2018 年 12 月 17−18 日.
10. 「同位体シフトで探る素粒子の新しい相互作用」、田中実（大阪大）、埼玉県和光市、2019 年 1 月 24 日（第 26 回核分光研 & 新学術領域研究「量子ビーム応用 」B03 合同セミナー）
11. 第 10 回 停止・低速不安定核ビームを用いた核分光研究会、福岡県福岡市、2019 年 3 月 18−19 日
12. 「計算機を活用した固体 NMR の解析法」、藤山茂樹（理研）、埼玉県和光市、2019 年 7 月 24 日（第 27 回核分光研 & 新学術領域研究「量子ビーム応用 」B03 合同セミナー）

13. 静周期磁場によるポジトロニウム超微細構造の観測実験」、永田祐吾 （東京理科大）、埼玉県和光市、2019 年 11 月 5 日（第 28 回核分光研 & 新学術領域研究「量子ビーム応用 」A01/B03 合同セミナー）
14. 「極低温 Fr 原子を用いたパリティ非保存効果誘起の光シフトの研究： 標準模型を超えた新物理と核のアナポールモーメント」、青木貴稔氏（東京大学）、埼玉県和光市、2019 年 12 月 20 日（第 29 回核分光研 & 新学術領域研究「量子ビーム応用 」B03 合同セミナー）
15. 第 11 回 停止・低速不安定核ビームを用いた核分光研究会、大阪府泉南郡熊取町、2020 年 1 月 16−17 日
16. 第 3 回若手放談会：エキゾチック核物理の将来、兵庫県神戸市、2020 年 2 月 19−21 日
17. “Er-implanted silica lasers based on Si nanobeam cavities,” 山下大喜氏（理研光量子工学研究センター量子オプトエレクトロニクス研究チーム）、埼玉県和光市、2020 年 2 月 27 日（第 30 回核分光研 & 新学術領域研究「量子ビーム応用 」B03 合同セミナー）

(8) Awards and honors

N/A

(9) Press releases

1. 理研プレスリリース、「ジルコニウム同位体は励起状態でも突然変形する」、2020 年 3 月 17 日. https://www.riken.jp/press/2020/20200317_2/index.html
2. 東京大学&理研共同記者発表、「原子核の形の基本原理と量子系での自己組織化」、2019 年 11 月 26 日. https://www.riken.jp/press/2019/20191126_1/index.html
3. 理研＆東大共同記者発表、「磁気モーメントから分かる銅同位体の新たな姿 －極限までスピン整列度を高めた RI ビームを駆使して測定に成功－」、2019 年 1 月 30 日. https://www.riken.jp/press/2019/20190130_2/
4. 日本経済新聞オンライン、「理研と東大など、中性子過剰な銅同位体原子核の励起状態の磁気モーメント測定に成功」、2019 年 1 月 30 日.
5. 東大＆理研共同記者発表、「水銀原子核はハムレット」、2018 年 10 月 2 日. https://www.riken.jp/press/2018/20181002_1/index.html
6. 東大＆理研共同記者発表、「原子核形状の２次相転移をスパコンシミュレーションで発見」、2018 年 8 月 13 日. https://www.riken.jp/press/2018/20180813_1/index.html

Atomic, Molecular and Optical Physics Laboratory
東原子分子物理研究室

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Toshiyuki AZUMA Chief Scientist RIKEN Cluster for Pioneering Research Atomic, Molecular and Optical Physics Laboratory 2-1 Hirosawa Wako Saitama 351-0198 JAPAN +81-(0)48-462-1614 toshiyuki-azuma@riken.jp 
Education	1983-1988 Graduate School of Engineering, The University of Tokyo 1981-1983 The University of Tokyo, Faculty of Engineering, Department of Nuclear Engineering 1979-1981 The University of Tokyo, College of General Education
Degrees	Dr. Eng. (1988) The University of Tokyo M. Eng. (1985) The University of Tokyo B. Eng. (1983) The University of Tokyo
Employment/research experience	2009- Atomic, Molecular and Optical Physics Laboratory, RIKEN 2005-2009 Professor, Department of Physics, Tokyo Metropolitan University 2000-2005 Associate Professor, Department of Applied Physics, Tokyo Metropolitan University 1998-2000 Associate Professor, Department of Physics, University of Tsukuba 1989-1998 Research Associate, Institute of Physics, University of Tokyo 1988-1989 Post-Doc. Swiss Federal Institute of Technology and Univ. of Zürich <u>Additional post</u> 2009- Visiting Professor, Tokyo Metropolitan University 2019 Visiting Professor, Tohoku University 2017- Visiting Professor, Rikkyo University
Awards and honors	
Academic activities	Member; Atomic Collision Society of Japan President; Atomic Collision Society of Japan (2017) Member; Physical Society of Japan Member; The Japan Society of Applied Physics Vice-President; IUPAP (International Union of Pure and Applied Physics) (2017) Chair, C-15 commission (Atomic, Molecular, and Optical Physics) of IUPAP (2017) Member; Organizing Committee of International Symposium on Novel Electronic States in Molecular Conductors (1994) Member; International Advisory Committee of International Conference on the Physics of Highly Charged Ions (HCI) (2018, 2020) Member; International Program Advisory Board of International Workshop on Electrostatic Storage Devices (ESD) (2017, 2019)

	Member; General Committee of Asian International Seminar on Atomic and Molecular Physics (AISAMP) (2018, 2020) Member; International Committee of International Seminar on Ion-Atom Collisions (ISIAC) (2017, 2019) Member; International Committee of Symposium on Electron, Photon, and Ion Collisions on Molecular & Atomic Nanostructures (EPIC-MAN) (2019) Member; International Scientific Committee of International Conference on Atomic Collisions in Solids (ICACS) (2018)

(1) Participants

Toshiyuki Azuma（東俊行）	主任研究員
Susumu Kuma（久間晋）	専任研究員
Yuji Nakano（中野祐司）	専任研究員
Naoki Kimura（木村直樹）	研究員
Shinji Okada（岡田信二）	協力研究員
Sebastian Menk	特別研究員
Kiattichart Chartkunchand	特別研究員
Yasuhiro Ueno（上野恭裕）	特別研究員
Preeti Mishra	特別研究員
Takuya Okumura（奥村拓馬）	特別研究員
Paul Bertier	IPA
Masatomi Iizawa（飯澤 正登実）	JRA
Haruo Shiromaru（城丸春夫）	客員研究員（都立大学）
Hajime Tanuma （田沼肇）	客員研究員（都立大学）
Shinya Yamada（山田真也）	客員研究員（都立大学）
Tadashi Hashimoto（橋本直）	客員研究員（JAEA）

(2) Original papers（Research Category in [ ]）

1. S. Kuma and T. Azuma: “Pulsed Beam of Extremely Large Helium Droplets”, Cryogenics **88**, 78-80 (2017). [3]
2. Keisuke Hirata, Keishiro Yamashita, Satoru Muramatsu, Shinjiro Takano, Keijiro Ohshimo, Toshiyuki Azuma, Ryuzo Nakanishi, Takashi Nagata, Seiji Yamazoe, Kiichirou Koyasu and Tatsuya Tsukuda: “Anion photoelectron spectroscopy of free $[Au_{25}(SC_{12}H_{25})_{18}]^-$ ”, Nanoscale, **9**, 13409-13412 (2017). [3]
3. Y. Nakano, Y. Enomoto, T. Masunaga, S. Menk, P. Bertier and T. Azuma: “RICE: RIken Cryogenic Electrostatic ion storage ring", Rev. Sci. Instrum. **88**, 033110 (2017). [1,2]
4. N. Kono, R. Suzuki, T. Furukawa, J. Matsumoto, H. Tanuma, H. Shiromaru, T. Azuma and K. Hansen: “Electronic and vibrational radiative cooling of the small carbon clusters C_4^- and C_6^-”, Phys. Rev. A **98**, 06343 (2018). [1,2]
5. S. Menk, P. Bertier, Y. Enomoto, T. Masunaga, T. Majima, Y. Nakano, and T. Azuma: “A cryogenic linear ion trap beamline for providing keV ion bunches”, Rev. Sci. Instrum. **89**, 113110 (2018). [1]
6. Linda Feketeová, Paul Bertier, Thibaud Salbaing, Toshiyuki Azuma, Florent Calvo, Bernadette Farizon, Michel Farizon and Tilman D. Märk: “Impact of a hydrophobic molecular ion in the early stage of cloud formation”, PNAS **116**, (45) 22540-22544 (2019). [3]
7. Friedrich Aumayr, Kiyoshi Ueda, Emma Sokell, Stefan Schippers, Hossein Sadeghpour, Frederic Merkt, Thomas F Gallagher, F Barry Dunning, Paul Scheier, Olof Echt, Tom Kirchner, Stephan Fritzsche, Andrey Surzhykov, Xinwen Ma, Roberto Rivarola, Omar Fojon, Lokesh Tribedi, Emily Lamour, José R Crespo López-Urrutia, Yuri A Litvinov, Vladimir Shabaev, Henrik Cederquist, Henning Zettergren, Marika Schleberger, Richard A Wilhelm, Toshiyuki Azuma, Philippe Boduch, Henning T Schmidt and Thomas Stöhlker: “Roadmap on photonic, electronic and atomic collision physics: III. Heavy particles: with zero to relativistic speeds”, J. Phys. B **52**, 171003 (2019). [1,2]
8. FQ. Chen, N. Kono, R. Suzuki, T. Furukawa, H. Tanuma, P. Ferrari, T. Azuma, J. Matsumoto, H. Shiromaru, V. Zhaunerchyk, K. Hansen: “Radiative cooling of cationic carbon clusters, C_N^+, N = 8, 10, 13 and 16”, Phys. Chem. Chem. Phys. **21**, 1587 (2019). [2]
9. Y. Nakano, R. Igosawa, S. Iida, S. Okada, M. Lindley, S. Menk, R. Nagaoka, T. Hashimoto, S. Yamada, T. Yamaguchi, S. Kuma, T Azuma: “X-ray spectroscopy of muonic atoms isolated in vacuum with transition edge sensors”, JPS Conf. Proc., in press. [1,2]

(3) Reviews and books（ Research Category in [ ] ）

1. 城丸春夫、東俊行、古川武：“静電型イオン蓄積リングを用いた原子分子物理（II）輻射冷却の分子科学” 、原子衝突学会誌“しょうとつ」解説、2018 年第 **15** 巻第 1 号. [2]

2. 東俊行：“粒子ビームサイエンスの進歩と展望-HIMAC の成果を中心に- 6 章 [原子分子] HIMAC が切り拓いた高エネルギーイオン原子衝突の最前線、6.1 HIMAC が切り拓いた高エネルギーイオン原子衝突の最前線” 、RADIOISOTOPES、**68**、83–487 (2019). [1]
3. 東俊行、小牧研一郎：“粒子ビームサイエンスの進歩と展望-HIMAC の成果を中心に- 6 章 [原子分子] HIMAC が切り拓いた高エネルギーイオン原子衝突の最前線、6.2.1 数百 MeV/u 重イオンと固体標的 -X 線および二次電子放出-”、RADIOISOTOPES、**68**、489–499 (2019). [1]
4. 東俊行、中野祐司： “粒子ビームサイエンスの進歩と展望-HIMAC の成果を中心に- 6 章 [原子分子] HIMAC が切り拓いた高エネルギーイオン原子衝突の最前線, 6.2.2 数百 MeV/u 重イオンと結晶標的 I -2 次元コヒーレント共鳴励起-”、RADIOISOTOPES、**68**、501–515 (2019). [1]
5. 中野祐司、東 俊行：“粒子ビームサイエンスの進歩と展望-HIMAC の成果を中心に- 6 章 [原子分子] HIMAC が切り拓いた高エネルギーイオン原子衝突の最前線 6.2.3 数百 MeV/u 重イオンと結晶標的 II -3 次元コヒーレント共鳴励起-”、RADIOISOTOPES、**68**、517–528 (2019). [1]

(4) Invited presentations（ Research Category in [ ] ）

1. T. Azuma: “Detection of recurrent fluorescence photons”, 7th International Workshop on Electrostatic Storage Devices, (ESD2017), Lyon, France, Jun. (2017). [2]
2. T. Azuma: “AMO PHYSICS: Diversity and Specialty”, IUPAP (International Union of Pure and Applied Physics) Workshop “New Challenges in Pure and Applied Physics”, at 29th General Assembly, San Paulo, Brazil, Oct. (2017). [1,2,3]
3. Y. Nakano: “Status of the Laser Spectroscopy and Merged-beam Experiments at RICE ”, 10th International Conference on Nuclear Physics at Storage Rings (STORI’17), Kanazawa, Japan, Nov. (2017). [1,2]
4. T. Azuma: “Recurrent fluorescence observed with an ion storage ring”, 7th Topical Conference of the Indian Society of Atomic and Molecular Physics (ISAMP-TC7), Tirupati, India, Jan. (2018). [2]
5. T. Azuma: “Excitation and De-excitation Dynamics of Matters: from Molecular Ions to Highly Charged Heavy Ions”, International Seminar on Atomic and Molecular Physics (AISAMP13), Mumbai, India, Dec. (2018). [1,2]
6. T. Azuma: “Superconducting TES calorimeter for atomic and molecular physics”, International Workshop on Atomic and Molecular Collisions, Udaipur, India, Dec. (2018). [1]
7. T. Azuma: “RIKEN cryogenic storage ring RICE”, 8th International Workshop on Electrostatic Storage Devices (ESD8), Tianjin, China, Aug. (2019). [1,2]
8. T. Azuma: “High precision spectroscopy of muonic X-rays with a superconducting TES detector at J-PARC”, J-PARC Symposium 2019 (J-PARC2019), Tsukuba, Japan, Sep. (2019). [1]
9. T. Azuma: “High precision spectroscopy and dynamics of atom/molecules related with astrophysics”, IPMU workshop “The cosmos at high energies”, IPMU Univ. of Tokyo, Kashiwa, Japan, Oct. (2019). [1]
10. 東俊行: “10 GeV から meV までのエネルギースケールで原子分子の量子状態を制御し観測する”、 第 19 回多元研研究発表会、東北大学、2019 年 12 月. [1,2,3]
11. 東俊行: “TES 超伝導 X 線検出器が切り拓くミュオンビーム元素分析の展望”, 第 2 回文理融合シンポジウム量子ビームで歴史を探る-加速器が紡ぐ文理融合の地平-、大阪大学、2019 年 12 月. [1]

(5) Patent applications（ Research Category in [ ] ）

N/A

(6) Collaborations including both inside and outside project（ Research Category in [ ] ）

1. 東 俊行、Klavs Hansen （中国・天津大学）：分子励起状態の脱励起過程の理論研究 [2]
2. 東 俊行、Paul Indelicato（フランス・ソルボンヌ大学）：ミュオン原子エネルギー準位の QED 計算 [1]
3. 東 俊行、Thomas Stöhlker （ドイツ・GSI 重イオン科学研究所）：イオン蓄積リングを用いた多価イオン実験研究 [1]
4. 東 俊行、高橋忠孝 （東京大学）：負ミュオン分光の宇宙物理 X 線観測実験への応用 [1]

5. 東　俊行、三宅康博（愛媛大学）: J-PARC における負ミュオン分光実験研究 [1]
6. 東　俊行、長嶋泰之（東京理科大学）: 負ポジトロニウムのレーザー誘起電子脱離実験研究 [1]
7. 東　俊行、山口貴之　(埼玉大学) ：イオン蓄積リングによる分子イオン脱励起過程の研究 [2]
8. 東　俊行、中村信行（電気通信大学）: イオントラップ内多価イオン分光へのレーザーの応用 [1,2]

(7) Hosted seminars and symposiums

N/A

(8) Awards and honors

N/A

(9) Press releases

N/A

Surface and Interface Science Laboratory
Kim表面界面科学研究室

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Yousoo KIM Chief Scientist Surface and Interface Science Laboratory RIKEN Cluster for Pioneering Research 2-1 Hirosawa Wako Saitama 351-0198 JAPAN +81-(0)48-467-4073 ykim@riken.jp 
Education	1996-1999 Graduate School of Engineering, The University of Tokyo 1991-1993 Department of Chemistry, Graduate School of Natural Science, Seoul National University 1984-1991 College of Natural Science, Seoul National University
Degrees	Dr. Eng. (1999) The University of Tokyo M. Sci. (1993) Seoul National University B. Sci. (1991) Seoul National University
Employment/research experience	2015- Chief Scientist, Surface and Interface Science Laboratory, RIKEN 2010-2015 Associate Chief Scientist, Surface and Interface Science Laboratory, RIKEN 2006-2009 Senior Research Scientist, Surface Chemistry Laboratory, RIKEN 2002-2006 Research Scientist, Surface Chemistry Laboratory, RIKEN 1999-2002 Special Postdoctoral Researcher, Surface Chemistry Laboratory, RIKEN <u>Additional post</u> 2019- Adjunct Professor, Seoul National University, Korea 2018- Adjunct Professor, GIST, Korea 2018- Visiting Professor, Univ. of the Philippines Diliman, Philippines 2017- Visiting Professor, Kyushu University 2011- Visiting Professor, Saitama University 2008- Visiting Professor, Tokyo Institute of Technology
Awards and honors	Academic Award (Chemical Society of Japan) (2019) Nanoprobe Prize (Japan Science and Technology Agency) (2018) Commendation for Science and Technology by the MEXT (MEXT) (2018) International Academic Prize (Japan Society of Molecular Science) (2016) Sir Martin Wood Prize (Millennium Science Forum) (2009) Young Scientist Award (The Physical Society of Japan) (2008)
Academic activities	Member; Chemical Society of Japan Member; Physical Society of Japan Member; American Physical Society Member; The Surface Science Society of Japan Member; The Japan Society of Applied Physics Member; Japan Society of Molecular Science Member; The Adhesion Society of Japan

(1) Participants

Yousoo Kim（金 有洙）	主任研究員
Norihiko Hayazawa（早澤 紀彦）	専任研究員
Yasuyuki Yokota（横田 泰之）	専任研究員
Hiroshi Imada（今田 裕）	上級研究員
Emiko Kazuma（數間 惠弥子）	研究員
Shunji Yamamoto（山本 駿玄）	研究員
Rafael Jaculbia	基礎特別研究員
Chi Zhang	基礎特別研究員
Misun Hong	基礎特別研究員
Qianchun Weng	基礎特別研究員
Kensuke Kimura（木村 謙介）	基礎特別研究員
Yena Kim	特別研究員
Catalan Francesca Celine Inserto	特別研究員
Chaunchaiyakul Songpol	特別研究員
Raymond Albert Wong	特別研究員
Miyabi Imada-Imai（今井 みやび）	特別研究員
Seungran Lee	協力研究員
Walen Holly Lynn	訪問研究員
Yang Bo	IPA（埼玉大学）
Inhae Zoh	IPA（Seoul National University, Korea）
Balgos Maria Herminia Marallag	IPA（University of the Philippines Diliman, The Philippines）
Ouyang Chun	IPA（東京工業大学）
Minhui Lee	JRA（東京大学）
Takuya Miyazaki（宮崎 拓也）	JRA（東京工業大学）
Lee Yea-Shine	実習生（Princeton University, USA）
Jaehyun Bae	研修生（九州大学）
Makoto Horikawa（堀川 聖）	研修生（横浜国立大学）
Yuta Morinaga（森永 悠太）	研修生（横浜国立大学）
Yoshitugu Shiro（城 宜嗣）	客員主管研究員（兵庫県立大学）
Susumu Komiyama（小宮山 進）	客員主管研究員（東京大学）
Jun Takeda（武田 淳）	客員主幹研究員（横浜国立大学）
Michael Trenary	客員主管研究員（University of Illinois at Chicago, USA）
Taro Yamada（山田 太郎）	客員主管研究員（東京大学）
Chihaya Adachi（安達 千波矢）	客員主管研究員（九州大学）
Kwon Jieon	客員主管研究員（Seoul National University, Korea）
Hajime Nakanotani（中野谷 一）	客員研究員（九州大学）
Ryuichi Arafune（荒船 竜一）	客員研究員（物質・材料研究機構）
Toshu An（安 東秀）	客員研究員（北陸先端科学技術大学院大学）
Yasuaki Einaga（栄長 泰明）	客員研究員（慶応大学）
Satoshi Katano（片野 諭）	客員研究員（東北大学）
Hiroyuki Kato（加藤 浩之）	客員研究員（大阪大学）
Abhishek Grewal	客員研究員（Max Planck Institute, Germany）
Izabela Irena Rzeznicka	客員研究員（芝浦工業大学）
Noriaki Takagi（髙木 紀明）	客員研究員（東京大学）
Ikufumi Katayama（片山 郁文）	客員研究員（横浜国立大学）
Emi Minamitani（南谷 英美）	客員研究員（分子科学研究所）
Tomohiro Hayashi（林 智広）	客員研究員（東京工業大学）
Masahiko Hara（原 正彦）	客員研究員（東京工業大学）
Takaaki Yano（矢野 隆章）	客員研究員（東京工業大学）
Kuniyuki Miwa（三輪 邦之）	客員研究員（Northwestern University, USA）
Ju-Hyung Kim	客員研究員（Ajou University, Korea)
Jaehoon Jung	客員研究員（University of Ulsan, Korea）

Hyunseob Lim 客員研究員（GIST, Korea）
Hye Ryung Byon 客員研究員（KAIST, Korea）
Chi Chen 客員研究員（Academia Sinca, Taiwan）

(2) Original papers（Research Category in [ ]）

1. H. Imada, K. Miwa, M. Imai-Imada, S. Kawahara, K. Kimura, and Y. Kim, "Single molecule investigation of energy dynamics in a coupled plasmon-exciton system", Phys. Rev. Lett., **119**, 013901, 1-6 (2017). [2]
2. F. C. Catalan, N. Hayazawa, Y. Yokota, R. Wong, T. Watanabe, Y. Einaga, and Y. Kim, "Facet-Dependent Temporal and Spatial Changes in Boron-Doped Diamond Film Electrodes due to Anodic Corrosion", J. Phys. Chem. C, **121**, 26742-26750 (2017) [1].
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9. S. Kim, C. Park, M. Lee, I. Song, J. Kim, M. Lee, J. Jung, Y. Kim, H. Lim, and H. C. Choi, "Rapid photochemical synthesis of sea-urchin-shaped hierarchical porous COF-5 and its lithography-free patterned growth", Adv. Funct. Mater., **27**, 1700925 (2017) [1].
10. H. W. Kim, W. Ko, J. Ku, Y. Kim, S. Park, and S. Hwang, "Evolution of Graphene Growth on Pt(111): From Carbon Clusters to Nanoislands", J. Phys. Chem. C, **121**, 25074-25078 (2017) [1].
11. M. Imai-Imada, H. Imada, K. Miwa, J. Jung, T. K. Shimizu, M. Kawai, and Y. Kim, "Energy-level alignment of a single molecule on ultrathin insulating film", Phys. Rev. B, **98**, 201403(R), 1-6 (2018) [4].
12. E. Kazuma, J. Jung, H. Ueba, M. Trenary, and Y. Kim, "STM studies of photochemistry and plasmon chemistry on metal surfaces", Prog. Surf. Sci., **93**, 146-162 (2018) [2,4].
13. R. A. Wong, Y. Yokota, M. Wakisaka, J. Inukai, and Y. Kim, "Discerning the redox-dependent electronic and interfacial structures in electroactive self-assembled monolayers", J. Am. Chem. Soc., **140**, 13672-13679 (2018) [4,1].
14. B. Yang, E. Kazuma, Y. Yokota, and Y. Kim, "Fabrication of sharp gold tips by three-electrode electrochemical etching with high controllability and reproducibility", J. Phys. Chem. C, **122**, 16950-16955 (2018) [4].
15. S. A. B. Vizcara, L. P. Lopez, J. Daniel E. Vasquez, M. Herminia M. Balgos, D. Hashizume, N. Hayazawa, Y. Kim, M. Tani, A. S. Somintac, A. A. Salvador, and E. S. Estacio, "Intense THz emission in high quality MBE-grown GaAs film with thin n-doped buffer", Opt. Mater. Express, **8**, 1463-1471 (2018) [5].
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Adsorbed on Cu(100) at Low Coverage: Characterization and Stability against Complexation", J. Phys. Chem. B, **122**, 963-971 (2018) [3].
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22. C. Zhang, E. Kazuma, and Y. Kim, "Atomic-scale visualization of the stepwise metal-mediated dehalogenative cycloaddition reaction pathways: competition between radicals and organometallic intermediates,", Angew. Chem. Int. Ed., **58**, 17736-17744 (2019) [4,1].
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24. K. Kimura, K. Miwa, H. Imada, M. Imai-Imada, S. Kawahara, J. Takeya, M. Kawai, M. Galperin, and Y. Kim, "Selective triplet exciton formation in a single molecule", Nature, **570**, 210-213 (2019) [4,2].
25. J. Park, J.-H. Kim, S. Bak, K. Tahara, J. Jung, M. Kawai, Y. Tobe, and Y. Kim, "On-surface evolution of meso-isomerism in two-dimensional supramolecular assemblies", Angew. Chem. Int. Ed., **58**, 9611-9618 (2019) [1,4].
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31. Y. Yokota, N. Hayazawa, B. Yang, E. Kazuma, F. C. Inserto Catalan, and Y. Kim, "Systematic assessment of benzenethiol self-assembled monolayers on Au(111) as a standard sample for electrochemical tip-enhanced Raman spectroscopy", J. Phys. Chem. C, **123**, 2953-2963 (2019) [4,1].
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35. R. B. Jaculbia, H. Imada, K. Miwa, T. Iwasa, M. Takenaka, B. Yang, E. Kazuma, N. Hayazawa, T. Taketsugu, and Y. Kim, "Single-molecule resonance Raman effect in a plasmonic nanocavity", Nat. Nanotechnol., **15**, 105-110 (2020) [4,2].

36. J.-G. Ahn, J. Bang, J. Jung, Y. Kim, and H. Lim, “Scanning tunneling microscopic investigations for studying conformational change of underlying Cu(111) and Ni(111) during graphene growth”, Surf. Sci., **693**, 121526 (2020) [3].
37. E. Kazuma, M. Lee, J. Jung, M. Trenary, and Y. Kim, “Single-molecule study of a plasmon-induced reaction for a strongly chemisorbed molecule”, Angew. Chem. Int. Ed., [DOI: 10.1002/anie.202001863]. [2,4]

(3) Reviews and books（ Research Category in [ ] ）

1. 今田裕、三輪邦之、今井みやび、河原祥太、木村謙介、金有洙：“走査トンネル顕微鏡発光分光法による分子間エネルギー移動の実空間計測”、表面科学、**38**、455-459 (2017). [2]
2. H. Imada and Y. Kim, “Real-space investigation of energy transfer with single-molecule luminescence and absorption spectroscopy,”, AAPPS Bulletin, 28, 3-8 (2018) [4,2]
3. 今田裕、三輪邦之、今井みやび、金有洙：“原子分解能でみる分子間エネルギー移動”、日本物理学会誌、**73**、303-307 (2018). [4,2]
4. E. Kazuma and Y. Kim, “Mechanistic studies of plasmon chemistry on metal catalysts”, Angew. Chem. Int. Ed., 58, 4800-4808 (2019) [2,4].
5. E. Kazuma and Y. Kim, “Scanning probe microscopy for real-space observations of local chemical reactions induced by localized surface plasmon”, Phys. Chem. Chem. Phys., 21, 19720-19731 (2019). [2,4]
6. 横田泰之、レイモンド A. ウォン、金有洙：“固体／液体界面の電気二重層を真空中で精密解析する”、自動車技術、**73**、116-117 (2019). [4]

(4) Invited presentations（ Research Category in [ ] ）

1. Y. Kim: “Real-space Investigation of intermolecular energy transfer and with an STM”, The 9th International Workshop on Nanoscale Spectroscopy and Nanotechnology (NSS-9), Gyeongju, Korea. Sep. (2017). [1,2]
2. Y. Kim: “Investigation of Energy Transfer and Conversion at a Single molecule with an STM”, AVS International Symposium and Exhibition, Tampa, USA, Nov. (2017). [1,2]
3. H. Imada: “Spectroscopic investigation of single molecule energy dynamics with a scanning tunneling microscope”, The 4th International Conference & Exhibition for Nanotechnology (NANOPIA 2017), Gyeonggi, Korea, Nov. (2017). [2]
4. N. Hayazawa: “Breaking the Classical Limit: From Micro-to Nano- Spectroscopy and its Temporal Control”, The 1st NIP-RIKEN Joint Research Workshop, Diliman, Philippines, Nov. (2017). [2]
5. N. Hayazawa: “Tip-enhanced Raman and THz-Raman spectroscopy”, The 8th International Conference on Terahertz Nanoscience, Okayama, Japan, Nov. (2017). [2]
6. 金有洙：“Real-space investigation of energy transfer, conversion and dissipation of a single molecule at solid surfaces”、日本化学会第 98 春季年会、兵庫県神戸市、2018 年 3 月. [1,2]
7. 早澤紀彦：“チップ増強ナノスペクトロスコピーの開拓と多様な環境への展開”、第 65 回応用物理学会春季学術講演会、東京都新宿区、2018 年 3 月. [2]
8. 金有洙：“近接場光を用いた単分子反応と分光”、日本化学会第 98 春季年会、兵庫県神戸市、2018 年 3 月. [1,2]
9. Y. Kim: “Energy conversion and transfer at a single molecule”, 2018 Korean Physical Society (KPS) Spring Meeting, Daejeon, Korea, Apr. (2018). [1,2,4]
10. 數間惠弥子：“プラズモン誘起化学反応の単一分子レベル研究”、東京大学生産技術研究所 光物質ナノ科学研究センター Nanoscience Seminar、東京都目黒区、2018 年 4 月. [2,4]
11. 數間惠弥子：“プラズモン誘起化学反応の単一分子レベル研究”、2018 年度電気化学会関東支部セミナー「先端計測技術による電極界面分析の新展開」、東京都目黒区、2018 年 4 月. [2,4]
12. Y. Kim: “STM investigation of energy conversion and transfer at a single molecule”, France-Japan workshop on optoelectronics & Photonics, Paris, France, May. (2018). [1,2,4]
13. N. Hayazawa: “Tip-enhanced nanospectroscopy beyond ambient”, The 26th International Conference on Raman Spectroscoy (ICORS 2018), Jeju, Korea, Aug. (2018). [4,2]

14. Y. Kim: “Single-molecule chemistry and spectroscopy with localized surface plasmon”, 14th International Conference on Atomically Controlled Surfaces, Interfaces and Nanostructures (ACSIN-14)＆26th International Colloquium on Scanning Probe Microscopy (ICSPM26), Sendai, Japan, Oct. (2018). [1,2,4]
15. N. Hayazawa: “The genealogy of tip-enhanced Raman spectroscopy”, 14th International Conference on Atomically Controlled Surfaces, Interfaces and Nanostructures (ACSIN-14) & 26th International Colloquium on Scanning Probe Microscopy (ICSPM26), Sendai, Japan, Oct. (2018). [4,2]
16. E. Kazuma: “STM investigation of reaction mechanisms for photochemistry and plasmon chemistry on metal”, The 3rd International Workshop on Advanced Nanoscience and Nanomaterials 2018, Fukuoka, Japan, Oct. (2018). [2,4]
17. Y. Kim: “Single-molecule chemistry and spectroscopy by near-field light”, 2019 Annual Meeting of the Physical Society of Taiwan, Hsinchu, Taiwan, Jan. (2019). [1,2,4]
18. Y. Yokota: “Developments of In Situ and Ex Situ Techniques for Microscopic Studies of Electrochemical Reactions at Aqueous Solution/Electro Interfaces”, IMS symposium "Water at interfaces 2018", Okazaki, Japan, Jan. (2019). [4,1]
19. Y. Kim: “Single-molecule chemistry and spectroscopy by near-field light”, Annual Meeting of the Physical Society of Taiwan, Hsinchu, Taiwan, Jan. (2019). [1,2,3,4]
20. Y. Yokota: “Developments of In Situ and Ex Situ Techniques for Microscopic Studies of Electrochemical Reactions at Aqueous Solution/Electro Interfaces”, IMS symposium "Water at interfaces 2018", Okazaki, Japan, Jan. (2019). [4,1]
21. Y. Yokota: “In Situ and Ex Situ Investigations of Electrochemical Interfaces”, International Symposium on Molecular Science 2019, Tokyo, Japan, Mar. (2019). [4,1]
22. 金有洙：“走査トンネル顕微鏡を用いた三重項励起子形成の単一分子計測”、日本化学会第 99 春季年会、兵庫県神戸市、2019 年 3 月. [1,2,3,4]
23. 金有洙：“Real-space investigation of energy transfer, conversion and dissipation of a single molecule at solid surfaces”、日本化学会第 99 春季年会、兵庫県神戸市, 2019 年 3 月. [1,2,3,4]
24. 今田裕：“走査トンネル顕微鏡を用いた発光/吸収分光の開発と応用”、日本物理学会第 74 回年次大会、福岡県福岡市、2019 年 3 月. [4,2]
25. 今田裕：“近接場光と単一分子の相互作用の原子スケール解析：単一分子の光マニピュレーションに向けて”、第 66 回応用物理学会春季学術講演会、東京都目黒区 、2019 年 3 月. [4,2]
26. 數間惠弥子：“走査型トンネル顕微鏡による単一分子化学反応の解析”、分子研研究会「単分子有機化学の挑戦」、愛知県岡崎市、2019 年 5 月. [2,4]
27. N. Hayazawa: “Raman going into sub-nanometer and multiple environments”, The 7th Taiwan International Symposium on Raman Spectroscopy (TISRS) and Taiwan Association of Raman Spectroscopy Summer School (TARS), Taipei, Taiwan, Jun. (2019). [2,3,5]
28. N. Hayazawa: “Subnanometer resolution STM-TERS beyond ambient”, 10th International Conference on Advanced Vibrational Spectroscopy (ICAVS10), Auckland, New Zealand, Jul. (2019). [2,3,5]
29. N. Hayazawa: “Sub-nanometric tip-enhanced Raman spectroscopy in multiple environments”, Nano Korea 2019, Ilsan, South Korea, Jul. (2019). [2,3,5]
30. Y. Yokota: “Novel approaches for microscopic understanding of electrochemical interfaces: in situ and ex situ techniques”, 2019 RIKEN-NCHU Joint Symposium, Taichung City, Taiwan, Aug. (2019). [1,2,4]
31. Y. Kim: “Single-molecule chemistry and spectroscopy at surfaces”, 2019 RIKEN-NCHU Joint Symposium, Taichung City, Taiwan, Aug. (2019). [1,2,3,4,5]
32. Q. Weng: “Terahertz nanoscopy of non-equilibrium carrier dynamics: A thermometric approach”, The 2019 Infrared Terahertz Quantum Workshop (ITQW), Ojai, USA, Sep. (2019). [2,5]
33. Y. Kim: “Single-molecule optical spectroscopy with STM”, Atomic Level Characterization (ALC), Kyoto, Japan, Oct. (2019). [1,2,3,4]
34. Y. Kim: “Single-molecule optical spectroscopy”, 704.WE-Heraeus-Seminar "Exploring the Limits of Nanoscience with Scanning Probe Methods", Bad Honnef, Germany, Oct. (2019). [1,2,3,4]
35. Y. Kim: “Single-molecule optical spectroscopy with a photon STM”, 19th International Conference on Solid Films and Surfaces, Hiroshima, Japan, Oct. (2019). [1,2,3,4]
36. Y. Kim: “Single-molecule chemistry and spectroscopy with a photon STM”, The Seventh

RIKEN-NCTU Symposium on Physical and Chemical Sciences, Hsinchu, Taiwan, Oct. (2019). [1,2,3,4]

37. Y. Kim: “Single-molecule Chemistry and Spectroscopy with a Scanning Tunneling Microscope”, International Symposium for Nano Science (ISNS), Osaka, Japan, Nov. (2019) [1,2,3,4]
38. Q. Weng: “Imaging hot-electron distribution in nanoscale electronic devices”, International School and Symposium on Nanoscale Transport and phoTonics (ISNTT2019), Kanagawa, Japan, Nov. (2019). [5,2]
39. R. B. Jaculbia: “Single molecule tip-enhanced Resonance Raman spectroscopy in low temperature environments”, Philippine-Japan Conference on Photonics and Optical materials, Quezon, Philippines, Dec. (2019). [4,2]
40. N. Hayazawa: “Development of nano-Raman and the challenge towards nano-THz”, Philippine-Japan Conference on Photonics and Optical materials, Quezon, Philippines, Dec. (2019). [5,2]
41. N. Hayazawa: “Single molecule Raman spectroscopy and imaging via tip-enhancement”, OptoX-NANO 2019, Okayama, Japan, Dec. (2019). [4,2]
42. H. Imada: “Plasmon-exciton coupling at an STM junction: fundamental and applications for spatially-resolved single-molecule spectroscopy”, 27th International Colloquium on Scanning Probe Microscopy (ICSPM27), Shizuoka, Japan, Dec. (2019). [4,2]
43. H. Imada: “STM study of exciton creation and annihilation in a single molecule”, The 81st Okazaki Conference "Forefront of Measurement Technologies for Surface Chemistry and Physics in Real-Space, k-Space, and Real-Time", Aichi, Japan, Dec. (2019). [4,2]
44. E. Kazuma: “Single molecule study of plasmon-induced chemical reactions”, The 81st Okazaki Conference "Forefront of Measurement Technologies for Surface Chemistry and Physics in Real-Space, k-Space, and Real-Time", Aichi, Japan, Dec. (2019). [2,4]
45. 金有洙:“単一分子におけるエネルギー移動・変換・散逸の実空間計測と制御”、第 58 回玉城嘉十郎教授記念 公開学術講演会 －界面を考えるー、京都市, 12 月 9 日 (2019). [1,2,3,4]
46. 木村謙介、三輪邦之、今田裕、今井みやび、河原祥太、竹谷純一、川合眞紀、マイケル ガルペリン、金有洙:“STM 発光分光法を用いた選択的な三重項励起子形成の単一分子計測”、第 48 回応用物理学会秋季学術講演会, 東京都千代田区, 2020 年 3 月. [4,2]
47. 數間恵弥子:“Nanoscale analysis and control of chemical reactions induced by Iocalized surface plasmon”、日本化学会第 100 春季年会、千葉県野田市、2020 年 3 月. [4,2]
48. 數間恵弥子:“光 STM を用いたプラズモン誘起化学反応の単一分子レベル解析”、表面真空学会関東支部の講演会、愛知県岡崎市、2020 年 4 月. [2,4]

(5) Patent applications（ Research Category in [ ] ）

N/A

(6) Collaborations including both inside and outside project（ Research Category in [ ] ）

1. 金 有洙、加藤 雄一郎（理研、ヘテロ界面）：分子吸着によるカーボンナノチューブの励起子制御 [5]
2. 金 有洙、東 俊行（理研、物質階層原理）：超高分解能単一分子振動分光 [4,2]
3. 金 有洙、前田 瑞夫（理研、ヘテロ界面）：自己組織化 DNA 単分子膜の界面研究 [4]
4. 金 有洙、城 宜嗣（兵庫県立大学、ヘテロ界面）：膜たんぱく質の界面研究 [4]
5. 金 有洙、栄長 泰明（慶応大学）：ホウ素ドープダイヤモンド電極表面の研究 [3]
6. 金 有洙、安達 千波矢（九州大学）：高効率単分子発光メカニズム研究 [2,4,5]
7. 金 有洙、福島 孝典（東京工業大学）：自己絶縁分子膜の開発 [1,4]
8. 金 有洙、Klaus Kern（Max Planck Institute）：単一分子励起子形成の制御 [4,2]
9. 金 有洙、武田 淳（横浜国立大学）：超高速単分子発光分光法の開発 [4,2]
10. 金 有洙、内山 真伸（理研、東京大学）：互変異性に基づく単分子発光スイッチング [2,4]
11. 金 有洙、武次 徹也（北海道大学）：単分子ラマンスペクトルの解析理論の開発 [4,2]
12. 金 有洙、三輪 邦之（Northwestern University）：単分子発光の解析理論の開発 [4,2]
13. 金 有洙、上羽 弘（富山大学）：近接場光による単分子励起メカニズムの解析 [4,2]
14. 金 有洙、Jaehoon Jung（University of Ulsan）：自己組織分子膜形成メカニズムの解析 [1,4]

(7) Hosted seminars and symposiums

1. “5th Ito International Research Center (IIRC) Conference, Forefront of Molecular Dynamics at Surfaces and Interfaces: from a single molecule to catalytic reaction”, Tokyo, Japan, November 20-23 (2017).
2. 「物質階層原理研究」&「ヘテロ界面研究」合同研究会、御殿場市、2019 年 5 月 10-11 日.

(8) Awards and honors

1. 今田 裕：“The 8th RIKEN Research Incentive Award”、理研、2017 年 3 月.
2. 木村 謙介：“講演優秀賞”、第 6 回 ナノスケール分子デバイス若手講演会、2017 年 3 月.
3. 木村 謙介：“講演奨励賞(スチューデント部門) ”、日本表面科学会、2017 年 5 月.
4. 今田 裕：“講演奨励賞(若手研究者部門) ”、日本表面科学会、2017 年 5 月.
5. 木村 謙介：“第 7 回 CSJ 化学フェスタ 優秀ポスター賞”、日本化学会、2017 年 10 月.
6. 木村 謙介：“優秀講演賞”、第 7 回 ナノスケール分子デバイス若手講演会、2018 年 1 月.
7. Emiko Kazuma：“Poster Award, Engineering Prize”, SPDR and FPR program screening subcommittee in RIKEN、2018 年 1 月.
8. 金 有洙：“平成 30 年度科学技術分野の文部科学大臣表彰”、文部科学省、2018 年 4 月.
9. 今田 裕：“理研梅峰賞”、理研、2018 年 6 月.
10. 金 有洙, 今田 裕：“ナノプローブテクノロジー賞”、日本学術振興会ナノプローブテクノロジー第 167 委員会、2018 年 7 月.
11. Emiko Kazuma：“Young Researcher Award”、ACSIN-14 & ICSPM26、2018 年 10 月.
12. Chi Zhang：“Young Researcher Award”、ACSIN-14 & ICSPM26、2018 年 10 月.
13. 金 有洙：“第 36 回学術賞”、日本化学会、2019 年 3 月.
14. 今田 裕：“日本物理学会若手奨励賞”、日本物理学会、2019 年 3 月.
15. 數間 恵弥子：“The 10th Research Incentive Award (桜舞賞) ”、理研、2019 年 3 月.
16. 今井 みやび：“学生優秀発表賞”、日本物理学会、2019 年 3 月.
17. 今井 みやび：“講演優秀賞”、第 8 回 ナノスケール分子デバイス若手講演会、2019 年 3 月.
18. 木村 謙介：“講演奨励賞(スチューデント部門) ”、日本表面真空学会、2019 年 5 月.
19. 數間 恵弥子：“平成 31 年度花王科学奨励賞”、公益財団法人花王芸術・科学財団、2019 年 6 月.
20. 今田 裕、三輪 邦之、今井 みやび、河原 祥太、木村 謙介、金 有洙：“日本表面真空学会会誌賞”、日本表面真空学会、2019 年 10 月.
21. 今井 みやび：“Poster Award”、27th International Colloquium on Scanning Probe Microscopy (ICSPM27)、2019 年 12 月.
22. Shunji Yamamoto：“Poster Award, Physics Prize”, SPDR and FPR program screening subcommittee in RIKEN、2020 年 1 月.
23. 木村 謙介：“総長賞”、東京大学、2020 年 3 月.
24. 木村 謙介：“研究科長賞”、東京大学新領域創成科学研究科、2020 年 3 月.
25. 木村 謙介：“第 47 回 応用物理学会講演奨励賞”、応用物理学会、2020 年 3 月.
26. 數間 恵弥子：“第 69 回進歩賞”、日本化学会、2020 年 3 月.

(9) Press releases

1. プレスリリース、“新原理に基づく単一分子発光・吸収分光を実現”、2017 年 7 月 5 日 https://www.riken.jp/press/2017/20170705_1/
2. 日本経済新聞、“理研、新原理に基づく単一分子発光・吸収分光を実現”、2017 年 7 月 5 日
3. プレスリリース、“ナノの光で起こる化学反応”、2018 年 5 月 4 日. https://www.riken.jp/press/2018/20180504_1/
4. Chemistry World、“Plasmon chemistry sheds new light on designing photocatalysts”、2018 年 5 月 5 日.
5. プレスリリース、“固体/液体界面の電気二重層を真空中で精密解析”、2018 年 11 月 12 日.

https://www.riken.jp/press/2018/20181112_1/index.html
6. 日本経済新聞、“理研、固体/液体界面の電気二重層の状態を溶液・真空中で精密に測定できる複合システムを開発”、2018 年 11 月 12 日.
7. プレスリリース、“単一分子電界発光の機構解明”、2019 年 3 月 1 日.
https://www.riken.jp/press/2019/20190301_1/
8. 日本経済新聞、“理研など、単一分子電界発光（エレクトロルミネッセンス）の機構を解明”、2019 年 3 月 1 日.
9. プレスリリース、“有機 EL の新たな発光機構を発見”、2019 年 6 月 6 日.
https://www.riken.jp/press/2019/20190606_1/
10. 日本経済新聞、“理研と東大など、有機 EL デバイスにおいて三重項励起子を低電圧で選択的に形成する新たな機構を発見”、2019 年 6 月 6 日.
11. プレスリリース、“単一分子による共鳴ラマン散乱の可視化に成功”、2020 年 2 月 17 日.
https://www.riken.jp/press/2020/20200217_1/index.html
12. プレスリリース、“ナノの光による単一酸素分子の分解”、2020 年 3 月 23 日.
https://www.riken.jp/press/2020/20200323_1/index.html

Molecular Spectroscopy Laboratory
田原分子分光研究室

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Tahei TAHARA Chief Scientist RIKEN Cluster for Pioneering Research Molecular Spectroscopy Laboratory 2-1 Hirosawa Wako Saitama 351-0198 JAPAN +81-(0)48-467-4592 tahei@riken.jp 
Education	1984-1989 Graduate School of Science, The University of Tokyo 1982-1984 The University of Tokyo, Faculty of Science, Department of Chemistry 1980-1982 The University of Tokyo, College of General Education
Degrees	Dr. Sci. (1989) The University of Tokyo M. Sci. (1986) The University of Tokyo B. Sci. (1984) The University of Tokyo
Employment/research experience	2001- Chief Scientist, Molecular Spectroscopy Laboratory, RIKEN 1995-2001 Associate Professor, Institute for Molecular Science (IMS) 1990-1994 Research Associate, Kanagawa Academy of Science and Technology (KAST) 1989-1990 Research Associate, Department of Chemistry, Faculty of Science, The University of Tokyo <u>Additional post</u> 2017-2020 Visiting Professor, Tokyo Institute of Technology 2017-2019 Distinguished Visiting Professor, Indian Institute of Technology, Bombay 2011-2015 Visiting Professor, Indian Institute of Technology, Bombay 2004- Visiting Professor, Saitama University 2003- 2006 Visiting Professor, The University of Tokyo 1995-2000 Associate Professor, Graduate University for Advanced Studies
Awards and honors	Mizushima-Raman Lecturer Award (2020) TRVS Lifetime Achievement Award (2019) Award for Outstanding Contribution to Raman Spectroscopy (2018) Distinguished Scientist Awards of the Japan Society for Molecular Science (2017) Spectroscopical Society of Japan Award (2017) MEXT Prizes for Science and Technology (2017) Distinguished Asian Visiting Speaker Award (2013) Chemical Society of Japan Award for Creative Work (2012) The JSPS Prize (2006) IBM Japan Science Prize (2004) TRVS Outstanding Young Researcher Award (2001) Morino Science Award (2000) Award of Research Foundation for Opto-Science and Technology (1995)
Academic activities	Member; Japan Society for Molecular Science

	Member; Chemical Society of Japan Member; Spectroscopical Society of Japan Member; American Chemical Society Editorial Advisory Board, Journal of Physical Chemistry Letters (2020-) Editorial Board, Journal of Chemical Physics (2013 - 2015). Advisory Editorial Board Member, Chemical Physics (2012 - present). Editorial Advisory Board, Journal of Physical Chemistry (2010 – 2012). Guest Editor, Chemical Physics and Physical Chemistry, Themed Issue on "Complex molecular systems: supramolecules, biomolecules and interfaces" (2017). Guest Editor, Chemical Physics, Special Issue on Edwin J. Heilweil (2017). International Steering Committee, Asian Spectroscopy Conference (ASC) (2015 -) International Steering Committee, International Conference on Raman Spectroscopy (ICORS) (2010 - 2016). International Advisory Committee, International Conference on Time-Resolved Vibrational Spectroscopy (TRVS) (2008 -). Chair, 16th International Conference on Time-Resolved Vibrational Spectroscopy (TRVS2013) (2013). Program Chair, Ultrafast Phenomena (2020). Chair, The 8th Asian Spectroscopy Conference (2021). President, Japan Society of Molecular Science (2018 - 2020). Head, Division of Advanced Laser Spectroscopy, Spectroscopical Society of Japan (2005 -). Advisory Committee, Institute for Molecular Science (2012 - 2016). Board, Spectroscopical Society of Japan (2014 - 2018). Head, Grant-in-Aid for Scientific Research on Innovative Areas (KAKENHI project), "Soft Molecular Systems," MEXT (2013-2018). Group Leader, Grant-in-Aid for Scientific Research on Priority Area (KAKENHI project), "Molecular Science for Supra Functional Systems," MEXT (2007-2012).

(1) Participants

Tahei Tahara（田原 太平）	主任研究員
Kunihiko Ishii（石井 邦彦）	専任研究員
Satoshi Nihonyanagi（二本柳 聡史）	専任研究員
Hikaru Kuramochi（倉持 光）	研究員
Bidyut Sarkar	特別研究員
Ahmed Mohammed	特別研究員
Pardeep Kumar	特別研究員
Woongmo Sung	特別研究員
Korenobu Matsuzaki（松﨑 維信）	基礎科学特別研究員
Tsukasa Takanashi（髙梨 司）	訪問研究員
Li Liu	特別研究員
Feng Wei	協力研究員
Wooseok Heo	訪問研究員
Atsushi Sayama（佐山 篤）	JRA
Haruko Hosoi（細井 晴子）	客員研究員（東邦大学）
Munetaka Iwamura（岩村 宗高）	客員研究員（富山大学）
Tatsuya Fujino（藤野 竜也）	客員研究員（東洋大学）
Anton Myalitsin	客員研究員（日産アーク）
Shoichi Yamaguchi（山口 祥一）	客員主管研究員（埼玉大学）
Masahisa Osawa（大澤 正久）	客員主管研究員（日本工業大学）
Satoshi Takeuchi（竹内 佐年）	客員主管研究員（兵庫県立大学）

(2) Original papers（Research Category in [ ]）

1. H. Kuramochi, S. Takeuchi, K. Yonezawa, H. Kamikubo, M. Kataoka and T. Tahara: “Probing the early stages of photoreception in photoactive yellow protein with ultrafast time-domain Raman spectroscopy”, Nat. Chem., **9**, 660- 666 (2017). [2]
2. T. Otosu, K. Ishii, H. Oikawa, M. Arai, S. Takahashi and T. Tahara: “Highly heterogeneous nature of the native and unfolded states of the B domain of protein A revealed by two-dimensional fluorescence lifetime correlation spectroscopy”, J. Phys. Chem. B, **121**, 5463-5473, (2017). [2]
3. W. Pao, K. Hanaoka, T. Fujisawa, S. Takeuchi, T. Komatsu, T. Ueno, T. Terai, T. Tahara: T. Nagano and Y. Urano: “Development of an Azo-based Photosensitizer Activated under Mild Hypoxia for Photodynamic Therapy”, J. Am. Chem. Soc., **139**, 13713–13719 (2017). [2]
4. K. Inoue, P. C. Singh, S. Nihonyanagi, S. Yamaguchi, and T. Tahara: “Cooperative hydrogen-bond dynamics at a zwitterionic lipid/water interface revealed by 2D HD-VSFG spectroscopy”, J. Phys. Chem. Lett., **8**, 20, 5160–5165 (2017). [4]
5. S. Tahara, S. Takeuchi, R. Abe-Yoshizumi, K. Inoue, H. Ohtani, H. Kandori and T. Tahara: “Origin of the reactive and non-reactive excited states in the primary reaction of rhodopsins: pH dependence of femtosecond absorption of light-driven sodium ion pump rhodopsin KR2”, J. Phys. Chem. B, **122**, 4784-4792 (2018). [2]
6. K. Inoue, S. Tahara, Y. Kato, S. Takeuchi, T. Tahara and H. Kandori: “Spectroscopic study of proton transfer mechanism of inward proton pump rhodopsin, Parvularcula oceani xenorhodopsin”, J. Phys. Chem. B, **122**, 6453-6461 (2018). [2]
7. S. Urashima, A. Myalitsin, S. Nihonyanagi and T. Tahara: “The topmost water structure at a charged silica/aqueous interface revealed by heterodyne-detected vibrational sum frequency generation spectroscopy”, J. Phys. Chem. Lett., **9**, 4109-4114 (2018). [4]
8. M. M. Sartin, W. Sung, S. Nihonyanagi and T. Tahara: “Molecular mechanism of charge inversion revealed by polar orientation of interfacial water molecules: A heterodyne-detected vibrational sum frequency generation study”, J. Chem. Phys., **149**, 024703 (2018). [4]
9. H. Kuramochi, S. Takeuchi, and T. Tahara: “Ultrafast photodissociation dynamics of diphenylcyclopropenone studied by time-resolved impulsive stimulated Raman spectroscopy”, Chem.

Phys. **512**, 88-92(2018). [2]

10. M. Iwamura, K. Kimoto, K. Nozaki, H. Kuramochi, S. Takeuchi and T. Tahara: "Metal–metal bond formations in $[Au(CN)_2^-]_n$ (n = 3–5) oligomers in water identified by coherent nuclear wavepacket motions", J. Phys. Chem. Lett., **9**, 7085–7089 (2018). [2]
11. K. Inoue, M. Ahmed, S. Nihonyanagi and T. Tahara: "Effect of hydrogen-bond on ultrafast spectral diffusion dynamics of water at charged monolayer interfaces", J. Chem. Phys., **150**, 054705/1-7 (2019). [4]
12. S. Tahara, M. Singh, H. Kuramochi, W. Shihoya, K. Inoue, O. Nureki, O. Béjà, Y. Mizutani, H. Kandori and T. Tahara: "Ultrafast dynamics of heliorhodopsins", J. Phys. Chem. B, **123**, 2507–2512 (2019). [2]
13. H. Kuramochi, S. Takeuchi, H. Kamikubo, M. Kataoka and T. Tahara: "Fifth-order time-domain Raman spectroscopy of photoactive yellow protein for visualizing vibrational coupling in its excited state", Sci. Adv., **5 (6)**, eaau4490 (2019). [2]
14. L. Wang, S. Nihonyanagi, K. Inoue, K. Nishikawa, A. Morita, S. Ye and T. Tahara: "Effect of frequency-dependent Fresnel Factor on the Vibrational Sum Frequency Generation Spectra for Liquid/Solid Interfaces," J. Phys. Chem. C (Hai-Lung Dai Festschirift), **123**, 15665−15673 (2019). [4]
15. K. Matsuzaki, S. Nihonyanagi, S. Yamaguchi, T. Nagata and T. Tahara: "Quadrupolar mechanism for vibrational sum frequency generation at air/liquid interfaces: Theory and experiment", J. Chem. Phys., **151**, 064701/1-15 (2019). [4]
16. B. Sarkar, K. Ishii and T. Tahara: "Microsecond conformational dynamics of biopolymers revealed by dynamic-quenching two-dimensional fluorescence lifetime correlation spectroscopy with single dye-labeling", J. Phys. Chem. Lett., **10**, 5536-5541 (2019). [2]
17. T. Otosu, K. Ishii and T. Tahara: "Multifocus fluorescence correlation spectroscopy with spatially separated excitation beams", Bull. Chem. Soc. Jpn., **92**, 1495-1502 (2019). [2]
18. S. Tahara, H. Kuramochi, S. Takeuchi and T. Tahara: "Protein dynamics preceding photoisomerization of the retinal chromophore in bacteriorhodopsin revealed by deep-UV femtosecond stimulated Raman spectroscopy", J. Phys. Chem. Lett., **10**, 5422-5427 (2019). [2]
19. S. Nihonyanagi, A. Sayama, Y. Ohshima and T. Tahara: "In-Situ Referencing method for heterodyne-detected vibrational sum frequency generation measurements at liquid/metal interfaces," Chem. Lett. **48**, 1387-1390 (2019). [4]
20. C. Chang, H. Kuramochi, M. Singh, R. Abe-Yoshizumi, T. Tsukuda, H. Kandori and T. Tahara: "Acid-base equilibrium of the chromophore counterion results in distinct Photoisomerization reactivity in the primary event of proteorhodopsin", Phys. Chem. Chem. Phys., **21**, 25728-25734 (2019). [2]
21. H. Kuramochi, S. Takeuchi, M. Iwamura, K. Nozaki and T. Tahara: "Tracking photoinduced Au-Au bond formation through transient terahertz vibrations observed by femtosecond time-domain Raman spectroscopy", J. Am. Chem. Soc., **141**, 19296-19303 (2019). [2]
22. A. Sayama, S. Nihonyanagi, Y. Ohshima and T. Tahara: "In situ observation of the potential-dependent structure of an electrolyte/electrode interface by heterodyne-detected vibrational sum frequency generation," Phys. Chem. Chem. Phys., **22**, 2580-2589 (2020). [4]
23. W. Sung, C. Müller, S. Hietzschold, R. Lovrinčić, N. P. Gallop, A. A. Bakulin, S. Nihonyanagi and T. Tahara: "Preferred Orientations of Organic Cations at Lead-Halide Perovskite Interfaces Revealed using Vibrational Sum-Frequency Spectroscopy", Mater. Horiz., in press (2020). [4]
24. M. Ahmed, K. Inoue, S. Nihonyanagi and T. Tahara: "Hidden isolated OH at the charged hydrophobic interface revealed by two-dimensional heterodyne-detected VSFG spectroscopy", Angew. Chem. Int. Ed., in press (2020). [4]

(3) Reviews and books（ Research Category in [ ] ）

1. S. Nihonyanagi, S. Yamaguchi and T. Tahara: "Ultrafast dynamics at water interfaces studied by vibrational sum-frequency generation spectroscopy", Chem. Rev., **117**, 10665-10693 (2017). [4]
2. 倉持光:"時間領域ラマン分光法の極限化とその光応答性タンパク質への応用"、分光研究、**66**、155 (2017). [2]
3. 石井邦彦、田原太平: "二次元分光法：タンパク質のダイナミクスを可視化する二次元蛍光寿命

相関分光法を中心として”、日本物理学会誌、**72**、854-861 (2017). [2]

4. S. Nihonyanagi and T. Tahara: “Vibrational Sum Frequency Generation Spectroscopy”, *In* Compendium of Surface and Interface Analysis, The Surface Science Society of Japan Ed., Springer, 801-807 (2018). [4]
5. 倉持光: “フェムト秒時間分解“時間領域”ラマン分光による光受容体初期構造ダイナミクスの実時間追跡”、光学、**47**、258 (2018). [2]
6. 倉持光、藤澤知績、竹内佐年、田原太平: “フェムト秒時間領域ラマン分光法を用いた光受容・発光タンパク質の反応ダイナミクスの研究”、生物物理、**59**、026-029 (2019). [2]
7. 坂口美幸: “IFCA（独立蛍光成分分析）の開発：生体分子の構造不均一性をモデルフリーで定量する方法”、生物物理、**59**、154-155 (2019). [2]
8. K. Inoue, S. Nihonyanagi and T. Tahara: “Ultrafast vibrational dynamics at aqueous interfaces studied by 2D heterodyne-detected vibrational sum frequency generation spectroscopy”, *In* Coherent Multidimensional Spectroscopy, Cho M. (eds), Springer Series in Optical Science book Series vol. **226**, Chap. 10, 215-236 (2019). [4]

(4) Invited presentations（ Research Category in [ ] ）

1. 倉持光：“時間領域ラマン分光法の極限化とその光応答性タンパク質への応用” 、平成 29 年度日本分光学会年次講演会、東京都新宿区、2017 年 5 月. [2]
2. 井上賢一：“ヘテロダイン検出振動和周波発生分光法を用いた界面水の超高速ダイナミクス”、分子研研究会「水の局所構造・物性解析の最先端」、愛知県岡崎市、2017 年 6 月. [4]
3. 田原太平： “新しい分光計測の開発と応用による複雑分子系ダイナミクスの研究”、東京工業大学理学院化学系 講演会、東京都目黒区、2017 年 6 月. [2,4]
4. 田原太平：“二次元蛍光寿命相関分光によるタンパク質のマイクロ秒ダイナミクスの研究”、シンポジウム：蛋白質の柔らかさと機能　Flexibility and function of proteins、第 17 回日本蛋白質科学会年会、宮城県仙台市、2017 年 6 月. [2]
5. T. Tahara: “Femtosecond nuclear dynamics of photo-induced structural changes of metal complexes”, 22nd International Symposium on Photochemistry and Photophysics of Coordination Compounds (ISPPCC 2017), Oxford, UK, Jul. (2017). [2]
6. S. Takeuchi, H. Kuramochi, M. Iwamura, K. Nozaki, T. Tahara: “Ultrafast time-domain Raman study of bond strengthening in oligomers of Au(I) complex”, International Conference on Time-Resolved Vibrational Spectroscopy (TRVS2017), Cambridge, UK, Jul. (2017). [2]
7. T. Tahara: “Ultrafast dynamics at water interfaces studied by time-resolved HD-VSFG”, The International Workshop on Nonlinear Optics at Interfaces, Dalian, China, Jul. (2017). [4]
8. T. Tahara: “Tracking structural dynamics of complex molecules by femtosecond time-domain Raman spectroscopy”, Telluride Science Research Center (TSRC) Workshop “Vibrational Dynamics”, CO, USA, Jul. (2017). [2]
9. K. Ishii, T. Tahara: “Development and application of two-dimensional fluorescence lifetime correlation spectroscopy”, The 6th Asian Spectroscopy Conference (ASC2017), Hsinchu, Taiwan, Sep. (2017). [2]
10. T. Tahara: “Ultrafast dynamics at water interfaces revealed by time-resolved heterodyne-detected vibrational sum-frequency generation”, The 6th Asian Spectroscopy Conference, Hsinchu, Taiwan, Sep. (2017). ***Keynote*** [4]
11. H. Kuramochi, S. Takeuchi, M. Iwamura, K. Nozaki, T. Tahara: “Capturing structural snapshots of tight Au-Au bond formation in [$Au(CN)_2^-$] oligomers by ultrafast time-domain Raman spectroscopy”, The 6th Asian Spectroscopy Conference, Hsinchu, Taiwan, Sep. (2017). [2]
12. 二本柳聡史：“新しい非線形分光法による固液界面の分子科学”、富山大学工学部セミナー、富山県富山市、2017 年 11 月. [4]
13. 浦島周平、二本柳聡史、田原太平：“シリカ/水溶液界面におけるヘテロダイン検出振動和周波発生分光：シリカ表面のプロトン化状態と最表面水構造”、若手研究者による先端的レーザー分光シンポジウム、埼玉県さいたま市、2017 年 12 月. [4]
14. T. Tahara: “Primary process of photo-responsive proteins studied by femtosecond time-domain Raman spectroscopy”, DAE - BRNS Trombay Symposium on Radiation & Photochemistry, Mumbai, India, Jan. (2018). ***Plenary*** [2]

15. T. Tahara: “Femtosecond dynamics of photo-induced structural changes of metal complexes”, Department Seminar, Department of Chemistry, Indian Institute of Science Education and Research (IISER) Bhopal, Bhopal, India, Jan. (2018). [2]
16. H. Kuramochi, S. Takeuchi, M. Iwamura, K. Nozaki, T. Tahara: “Direct observation of ultrafast structural dynamics in [$Au(CN)_2^-$] oligomers upon photo-induced tight Au-Au bond formation”, The 10th Asian Conference on Ultrafast Phenomena (ACUP 2018), Hong Kong, Jan. (2018). [2]
17. T. Tahara: “Novel single-molecule spectroscopy: microsecond structural dynamics of protein, DNA and RNA revealed by two-dimensional fluorescence lifetime correlation spectroscopy (2D-FLCS)”, Department Seminar, Department of Chemistry, Indian Institute of Technology (IIT) at Bombay, Mumbai, India, Jan. (2018). [2]
18. 倉持光：“時間領域ラマン分光法で観る分子の超高速構造ダイナミクス”、理研 研究員会議・分野横断ワークショップ、静岡県浜松市、2018 年 1 月. [2]
19. 倉持光：“超高速時間領域ラマン分光法で観る光応答性タンパク質のフェムト秒構造ダイナミクス”、レーザー学会学術講演会第 38 回年次大会、京都府京都市、2018 年 1 月. [2]
20. T. Tahara: “Femtosecond time-domain Raman spectroscopy”, Symposium on “90 Years of Raman Effect: Current Status and Future Direction”, Bangalore, India, Feb. (2018). [2]
21. T. Tahara: “Ultrafast primary process of photo-responsive proteins revealed by femtosecond Raman spectroscopy”, 255th ACS National Meeting & Exposition, Symposium: Ultrafast Spectroscopy Meets Chemistry, Materials and Biology (ANYL), LA, USA, Mar. (2018). [2]
22. K. Ishii: “Microsecond biomolecular dynamics observed at the single molecule level using two-dimensional fluorescence lifetime correlation spectroscopy”、日本化学会第 98 回春季年会アジア国際シンポジウム, 船橋市, 日本, Mar. (2018). [2]
23. T. Tahara: “Structural dynamics of photoresponsive proteins by femtosecond time-domain Raman spectroscopy”, Les Houches-TSRC Workshop “Protein Dynamics”, Les Houches, France, May (2018). [2]
24. T. Tahara: “Heterodyne-detected vibrational sum-frequency generation spectroscopy at buried aqueous interfaces”, Telluride Science Research Center (TSRC) Workshop “Nonlinear Optics at Interfaces”, Colorado, USA, Jun. (2018). [4]
25. T. Tahara: “Ultrafast vibrational dynamics at lipid/ water interfaces studied by 2D HD-VSFG spectroscopy”, The 9th International Conference on Coherent Multidimensional Spectroscopy (CMDS 2018), Seoul, Korea, Jun. (2018). [4]
26. T. Tahara: “Ultrafast vibrational dynamics at aqueous interfaces studied by 2D HD-VSFG spectroscopy”, Telluride Science Research Center (TSRC) Workshop “Advances of Multidimensional Vibrational Spectroscopy in Water, Biology and Materials Science”, Colorado, USA, Jul. (2018). [4]
27. T. Tahara: “Microsecond dynamics of biomolecules revealed by two-dimensional fluorescence lifetime correlation spectroscopy”, Telluride Science Research Center (TSRC) Workshop “Biophysical Dynamics”, Colorado, USA, Jul. (2018). [2]
28. T. Tahara: “Structure and dynamics of liquid interfaces studied by heterodyne-detected vibrational sum-frequency generation”, Gordon Research Conference 2018 Vibrational Spectroscopy, Biddeford, ME, USA, Jul. (2018). [4]
29. T. Tahara: “Femtosecond time-domain Raman spectroscopy”, The 26th International Conference on Raman Spectroscopy (ICORS 2018), Jeju, Korea, Aug. (2018). ***Plenary*** [2]
30. 田原太平：“Ultrafast structural dynamics of photoreceptor proteins revealed by femtosecond Raman spectroscopy フェムト秒ラマン分光による光受容タンパク質の超高速構造ダイナミクスの観測”、第 56 回日本生物物理学会年会、岡山県岡山市、2018 年 9 月. [2]
31. 坂口美幸、石井邦彦、田原太平、“一分子時間分解 FRET データの三次元解析：生体高分子の構造不均一性をモデルフリーで定量する方法の開発”、第 56 回日本生物物理学会年会、岡山県岡山市、2018 年 9 月. [2]
32. S. Takeuchi: “Ultrafast time-domain Raman approach to probe initial events in photoreception”, The 5th Ultrafast Dynamic Imaging of Matter (UFDIM), Agios Nikolaos, Greece, Sep. (2018). [2]
33. T. Tahara: “Catching ultrafast reactions at the water surface by femtosecond time-resolved HD-VSFG spectroscopy”, The 8th SFG Symposium, Omiya, Japan, Oct. (2018). [4]
34. S. Nihonyanagi: “HD-VSFG spectroscopic study of buried solid liquid interfaces”, The 8th SFG

Symposium, Omiya, Japan, Oct. (2018). [4]

35. B. Sarkar, K. Ishii, T. Tahara: “Observation of heterogeneous folding kinetics and distinct binding mechanisms of preQ1 riboswitch using two-dimensional fluorescence lifetime correlation spectroscopy (2DFLCS)”, Indo-Japan mini workshop “Frontiers in Molecular Spectroscopy: From Fundamentals to Applications in Chemistry and Biology”, Kobe, Japan, Oct. (2018). [2]
36. S. Takeuchi: “Ultrafast time-domain Raman study of bond strengthening in oligomers of Au(I) complex” Indo-Japan mini workshop “Frontiers in Molecular Spectroscopy: From Fundamentals to Applications in Chemistry and Biology”, Kobe, Japan, Oct. (2018). [2]
37. T. Tahara: “Structure and dynamics of water at the interface”, Joint Conference of EMLG/JMLG Meeting 2018 and 41st Symposium on Solution Chemistry of Japan, Nagoya, Japan, Nov. (2018). [4]
38. S. Nihonyanagi: “Phase-resolved Interface-selective Spectroscopy of Applied Interfaces”, 2nd International Workshop on Phase Interfaces for Highly Efficient Energy Utilization, Baltimore, USA, Nov. (2018). [4]
39. S. Nihonyanagi: “Structure and dynamics of liquid interfaces studied by phase- and time-resolved interface-selective nonlinear spectroscopies”, Seminar, Department of Chemistry, Temple University, Philadelphia, USA, Nov. (2018). [4]
40. 二本柳聡史：“Role of hydrogen bonding in ultrafast spectral diffusion dynamics of water at charged lipid interfaces”、分子研研究会「Water at interfaces」、愛知県岡崎市、2019 年 1 月. [4]
41. 坂口美幸： “二次元蛍光寿命相関分光法によるタンパク質の折りたたみ機構の研究と一分子 FRET データの新規解析法の開発”、理研シンポジウム「先端的レーザー分光の若手シンポジウム」、埼玉県和光市、2019 年 1 月. [2]
42. 田原太平 : “フェムト秒レーザーを用いた複雑な分子系の研究”、PF 研究会「高繰り返し極短パルス光源の未来」、茨城県つくば市、2019 年 1 月. [2,4]
43. T. Tahara: “Wonder world seen with light”, Institutional lecture, Indian Institute of Technology at Kanpur, Kanpur, India, Mar. (2019). [2,4]
44. M. Sakaguchi: “Development of IFCA (Independent Fluorescence Component Analysis): A method for quantification of heterogeneity with single-molecule time-resolved FRET data”, 43rd Indian Biophysical Society Meeting, Kolkata, India, Mar. (2019). [2]
45. 田原太平：“計測系から見た分子集合体の機能計測—超高速分光” 、シンポジウム「複雑系の分子科学－集まって立ち現れる分子機能の理解と設計」（日本化学会学術研究活性化委員会主催）、日本化学会第 99 春季年会、兵庫県神戸市、2019 年 3 月[2].
46. H. Kuramochi: “Ultrafast time-domain vibrational spectroscopy of complex molecular systems”, International Symposium on Molecular Science–Physical Chemistry/Theoretical Chemistry, Chemoinformatics, Computational Chemistry–Cosponsored by Japan Society for Molecular Science”, The 99th CSJ Annual Meeting, Kobe, Japan, Mar. (2019). [2]
47. M. Sakaguchi, “Observation of the site-specific compaction in the folding process of cytochrome c by two-dimensional fluorescence lifetime correlation spectroscopy”, Dept. of Chemical Sciences, Tata Institute of Fundamental Research, Mumbai, India, Mar. (2019). [2]
48. K. Ishii: “Multi-dimensional fluctuation analysis of FRET signals at the single-molecule level”, Dept. of Chemistry, University of Wisconsin-Madison, Madison, USA, Apr. (2019). [2]
49. 石井邦彦:“究極の一分子分光をめざして”、2019 年度日本分光学会年次講演会、京都府宇治市、2019 年 5 月. [2]
50. 二本柳聡史：“新規非線形分光法が解き明かす血液適合性高分子界面の構造”、理研・イブニングセミナー、東京、2019 年 6 月. [4]
51. T. Tahara: “Vibrational sum-frequency generation with quadrupole mechanism investigated by HD-VSFG spectroscopy”, International workshop on nonlinear optics at interfaces, Shanghai, China, Jun. (2019). [4]
52. T. Tahara: “Structural dynamics of chemical bond formation in the Au(I) complex oligomers revealed by femtosecond time-domain Raman spectroscopy”, International Conference on Ultrafast Structural Dynamics (ICUSD2019), Daejeon, Korea, Jun. (2019). [2]
53. T. Tahara: “Structural dynamics of bond formation in metal complex oligomers elucidated by femtosecond time-resolved impulsive stimulated Raman spectroscopy”, Telluride Science Research Center (TSRC) Workshop "Vibrational Dynamics", Colorado, USA, Jul. (2019). [2]

54. M. Iwamura, K. Nozaki, H. Kuramochi, S. Takeuchi, T. Tahara: “Nuclear wave-packet motions of metallophilic oligomers in solution”, 10th International Conference on Advanced Vibrational Spectroscopy (ICAVS 10), Auckland, New Zealand, Jul. (2019). [2]
55. S. Nihonyanagi: “Phase-resolved nonlinear spectroscopy at electrode/electrolyte solution interfaces”, 10th International Conference on Advanced Vibrational Spectroscopy (ICAVS 10), Auckland, New Zealand, Jul. (2019). [4]
56. H. Kuramochi, S. Takeuchi, M. Iwamura, K. Nozaki, T. Tahara: “Direct observation of ultrafast structural dynamics of the dicyanoaurate trimer upon photo-induced tight Au-Au bond formation”, 10th International Conference on Advanced Vibrational Spectroscopy (ICAVS 10), Auckland, New Zealand, Jul. (2019). [2]
57. T. Tahara: “Ultrafast dynamics at aqueous interface revealed by time-resolved HD-VSFG spectroscopy”, CECAM workshop on “Dynamics of Water in Complex Environments, Bridging the Gap between Molecular and Mesoscopic Interfaces”, Paris, France, Jul. (2019). [4]
58. T. Tahara: “Tracking ultrafast photochemical processes with observing excited-state coherent nuclear motion”, The 29th International Conference on Photochemistry (ICP 2019), Colorado, USA, Jul. (2019). [2]
59. T. Tahara: “Microsecond structural dynamics of bio-macromolecules revealed by two-dimensional fluorescence lifetime correlation spectroscopy”, Methods & Applications of Fluorescence (MAF 2019), California, USA, Aug. (2019). [2]
60. 田原太平、“挑戦したい幾つかの問題”、公益信託分子科学研究奨励森野基金　第 6 回森野ディスカッション、東京、2019 年 9 月. [2,4]
61. H. Kuramochi, T. Tahara: “Mapping ultrafast chemical reaction dynamics with femtosecond time-resolved time-domain Raman spectroscopy using few-cycle pulses”, 19th Time-Resolved Vibrational Spectroscopy Conference (TRVS2019), Auckland, New Zealand, Sep. (2019). [2]
62. A. Mohammed, S. Nihonyanagi, T. Tahara: “Vibrational spectra and ultrafast dynamics of interfacial water studied by steady-state and time-resolved HD-VSFG spectroscopy”, Indo-Japan workshop on “Frontiers in Molecular Spectroscopy: From Fundamentals to Applications in Chemistry and Biology”, Kobe, Japan, Oct. (2019). [4]
63. H. Kuramochi: “Mapping ultrafast chemical reaction dynamics with femtosecond time-resolved time-domain Raman spectroscopy”, Indo-Japan workshop on “Frontiers in Molecular Spectroscopy: From Fundamentals to Applications in Chemistry and Biology”, Kobe, Japan, Oct. (2019). [2]
64. T. Tahara: “Ultrafast dynamics at the water surface revealed by femotosecond interface-selective nonlinear spectroscopy”, Nature Conference on Functional Dynamics -Visualizing Molecules in Action-, Arizona, USA, Nov. (2019). ***Keynote*** [4]
65. T. Tahara: “Time-domain Raman spectroscopy and its application to ultrafast photochemical / photobiological reactions”, Mizushima Raman Lecture, 26th CRSI National Symposium in Chemistry (NSC-26), Vellore, India, Feb. (2020). [2]
66. T. Tahara: “Structure and dynamics at aqueous interface revealed by heterodyne-detected vibrational sum-frequency”, Department Seminar, Department of Inorganic and Physical Chemistry, Indian Institute of Science (IISc), Bangalore, India, Feb. (2020). [4]
67. T. Tahara: “Microsecond structural dynamics of protein, DNA and RNA revealed by two -dimensional fluorescence lifetime correlation spectroscopy (2D-FLCS)”, Department Seminar, Department of Chemistry, Indian Institute of Science Education and Research (IISER), Pune, India, Feb. (2020). [2]
68. T. Tahara: “Wonder world seen with ultrashort light”, Special Colloquium 2020, Pune, India, Feb. (2020). [2,4]
69. T. Tahara: “Structure and dynamics at aqueous interface revealed by heterodyne-detected vibrational sum-frequency”, Department Seminar, Department of Chemistry, Indian Institute of Technology at Bombay, Mumbai, India, Feb. (2020). [4]
70. T. Tahara: “Time-domain Raman spectroscopy and its application to ultrafast photochemical/ photobiological reactions”, Department Seminar, Department of Chemical Sciences, Tata Institute for Fundamental Research (TIFR), Mumbai, India, Feb. (2020). [2]
71. T. Tahara: “Wonder world seen with ultrashort light”, Mizushima-Raman Public Lecture, Delhi, India, Feb. (2020). [2,4]

72. T. Tahara: “Wonder world seen with ultrashort light”, Institute Lecture, Indian Institute of Science Education and Research (IISER) Bhopal, Bhopal, India, Feb. (2020). [2,4]
73. T. Tahara: “Structure and dynamics at aqueous interface revealed by heterodyne-detected vibrational sum-frequency”, Department Seminar, Department of Chemistry, Indian Institute of Science Education and Research (IISER) Bhopal, Bhopal, India, Feb. (2020). [4]
74. 倉持光:“超高速ラマン分光で観る光受容タンパク質におけるプロトン移動ダイナミクス”、TIA 連携プログラム探索事業「かけはし」量子反応シンポジウム、千葉県野田市、2020 年 3 月. [2]

(5) Patent applications（ Research Category in [ ] ）

1. 松崎維信、田原太平、石井邦彦：“分析方法、発光分析装置、拡散光トモグラフィー装置、撮像装置、反射率測定装置、分析装置、及びプログラム”、特願 2020-030796、2020 年 2 月 26 日. [2]

(6) Collaborations including both inside and outside project（ Research Category in [ ] ）

1. 田原 太平、石井 邦彦、廣田 俊（奈良先端科学技術大学院大学）：シトクロム c のフォールディング機構 [2]
2. 田原 太平、石井 邦彦、廣田 俊（奈良先端科学技術大学院大学）：シトクロム c の脂質二重膜との相互作用ダイナミクスの解明 [2]
3. 田原 太平、石井 邦彦、北尾 彰朗（東京工業大学）：実験と理論による DNA および RNA ヘアピンループの構造的差異の起源の解明 [2]
4. 田原 太平、石井 邦彦、飯野 亮太（分子科学研究所）：セルラーゼの構造不均一性とダイナミクス [2]
5. 田原 太平、石井 邦彦、Jayant Udgaonkar（インド国立生物科学センター）：プリオンタンパク質の天然状態ダイナミクス [2]
6. 田原 太平、石井 邦彦、Steve Pressé（アリゾナ州立大学）：ノンパラメトリックベイズ法を用いた蛍光寿命解析 [2]
7. 田原 太平、石井 邦彦、Randall Goldsmith（ウィスコンシン大学）：動電トラップを用いた溶液自由拡散分子の広時間領域一分子蛍光計測 [2]
8. 田原 太平、森田 明弘（東北大学）、石山 達也（富山大学）：実験と理論による水界面のプロトンの水和構造 [4]
9. 田原 太平、二本柳 聡史、森田 明弘（東北大学）、石山達也（富山大学）：水界面の二次非線形感受率スペクトルにおける変角振動バンドの出現機構 [4]
10. 田原 太平、二本柳 聡史、森田 明弘（東北大学）：長鎖アルキル単分子膜の二次非線形感受率スペクトルにおけるメチレン基の寄与 [4]
11. 田原太平、二本柳聡史、石山達也（富山大学）：アルコール単分子膜界面の二次非線形感受率スペクトルの理論解析 [4]
12. 田原 太平、二本柳 聡史、Artem Bakulin（Imperial College London）：ペロブスカイト薄膜界面の有機カチオンの配向解析 [4]
13. 田原 太平、二本柳 聡史、Artem Bakulin（Imperial College London）：蛍光および光電流測定による誘起電子材料中の振電相互作用の直接観測 [2]
14. 田原 太平、二本柳 聡史、青木隆史（京都工芸繊維大学）：生体適合性高分子の機能発現機構の解明 [4]
15. 田原 太平、二本柳 聡史、Anton Myalitsin（日産アーク）：和周波発生分光法の産業利用可能性の検討 [4]
16. 田原 太平、二本柳 聡史、前田瑞夫：ポリマーブラシ界面の構造解析 [4]
17. 田原 太平、二本柳 聡史、渋川雅美（埼玉大学）：エンドキャップした疎水性単分子膜界面の構造解析 [4]
18. 田原 太平、二本柳 聡史、八木一三（北海道大学）：白金/ナフィオン薄膜界面のスルフォン基の配向決定 [4]
19. 田原 太平、二本柳 聡史、Prashant Singh（Indian Association for the Cultivation of Science）：モデル生体膜界面への DNA の吸着挙動 [4]
20. 田原 太平、二本柳 聡史、候召 民（理研）：セルフヒーリングポリマー表面の構造解析 [4]

21. 田原 太平、倉持 光、武次 徹也（北海道大学）: スチルベン光異性化反応の超高速分光と ab initio MD 計算 [2]
22. 田原 太平、倉持 光、佐藤 治（九州大学）、坂本 章（青山学院大学）: 分極スイッチングを示す多核金属錯体の超高速分光[2]
23. 田原 太平、倉持 光、石井 邦彦、上野 秀樹、松尾 由賀利（法政大学）: 原子バブルの時間分解蛍光測定
24. 田原 太平、倉持 光、須藤 雄気（岡山大学）: ロドプシンの超高速分光 [2]
25. 田原 太平、倉持 光、神取 秀樹（名古屋工業大学）: ロドプシンの超高速分光 [2]
26. 田原 太平、倉持 光、井上 圭一（東京大学）: ロドプシンの超高速分光 [2]
27. 田原 太平、倉持 光、岩村 宗高（富山大学）、野崎 浩一（富山大学）: 遷移金属錯体の超高速分光 [2]
28. 田原 太平、倉持 光、水野 秀昭（KU Leuven）: 蛍光たんぱく質の超高速分光 [2]
29. 田原 太平、倉持 光、細井 晴子（東邦大学）: 蛍光たんぱく質の超高速分光 [2]
30. 田原 太平、倉持 光、Dongho Kim（Yonsei University）: π共役分子の超高速分光 [2]
31. 田原 太平、倉持 光、Eric Diau（National Chiao Tung University）: ペロブスカイトの超高速分光 [2]
32. 田原 太平、倉持光、Justin Hodgkiss（Victoria University of Wellington）: 生体関連色素の超高速分光 [2]

(7) Hosted seminars and symposiums

1. RIKEN Seminar, Prof. Michiel Sprik (University of Cambridge, UK.), “Electromechanics of the water liquid-vapour interface”, Wako, Saitama, 2019 年 4 月 16 日.
2. MSL Seminar, Ms. Bluebell Drummond (University of Cambridge, UK.), “The effects of molecular modification on intersystem crossing for improved thermally activated delayed fluorescence”, Wako, Saitama, 2019 年 9 月 24 日.
3. RIKEN Seminar, Prof. David M. Leitner (University of Nevada, Reno), “Energy Transport across Interfaces in Biomolecular Systems”, Wako, Saitama, 2019 年 10 月 21 日.
4. RIKEN Seminar, Prof. Sudipta Maiti (Tata Institute of Fundamental Research) , “In search of the elusive toxic oligomer in Amyloid diseases”, Wako, Saitama, 2019 年 12 月 5 日.
5. RIKEN Seminar, Prof. Eric Borguet (Temple University), “Impact of ions on structure and dynamics at aqueous interfaces”, Wako, Saitama, 2020 年 1 月 6 日.
6. MSL Seminar, Mr. M. Koga (Ph.D. student, Osaka University), “Direct Observation of Photoionization Dynamics in Solution Phase Induced by Simultaneous and Stepwise Two-Photon Excitation”, Wako, Saitama, 2020 年 3 月 18 日.

(8) Awards and honors

1. 田原 太平：“日本分光学会賞”、日本分光学会、2017 年 5 月 25 日.
2. 倉持 光：“平成 29 年度日本分光学会奨励賞”、日本分光学会、2017 年 5 月 25 日.
3. 田原 進也：“平成 29 年度日本分光学会年次講演会・優秀講演賞”、日本分光学会、2017 年 5 月 25 日.
4. Hikaru Kuramochi, Satoshi Takeuchi and Tahei Tahara: “Most Surprising Results Award”, The 13th Femtochemistry Conference, Cancun, Mexico, Aug.,2017.
5. 田原 太平：“第 8 回分子科学会賞”、分子科学会、2017 年 9 月 15 日.
6. 長谷川 一途：“第 11 回分子科学会優秀ポスター賞”、分子科学会、2017 年 11 月 1 日.
7. 田原 太平： “Outstanding Contribution to Raman Spectroscopy”, Indian Institute of Science, Bangalore, Mar., 2018.
8. 倉持 光：“日本化学会優秀講演賞（学術)”、日本化学会、2018 年 4 月 13 日.
9. Mohammed Ahmmed: “Best Poster Award”, 26th International Conference on Raman Spectroscopy,

Aug., 2018.

10. 坂口 美幸：“日本生物物理学会若手奨励賞”、日本生物物理学会、2018 年 9 月 16 日.
11. 倉持 光： “PCCP Prize”, Royal Society of Chemistry, Mar., 2019.
12. 田原 進也：“日本化学会 優秀講演賞（学術）”、日本化学会、2019 年 4 月 9 日.
13. 田原 太平：“TRVS Lifetime Achievement Award”, TRVS2019, Univ. Auckland, Nov., 2019.
14. 田原 太平：“Mizushima Raman Lecture Award”, Feb., 2020.
15. 倉持 光：“令和 2 年度文部科学大臣表彰（若手科学者賞）”、2020 年 4 月 14 日.
16. 倉持 光：“令和 2 年度分子科学研究奨励森野基金”、2020 年.

(9) Press releases

1. RIKEN RESEARCH News, “Lasers pick up good vibrations”, June 2, 2017.
   https://www.riken.jp/en/news_pubs/research_news/rr/20170001/index.html
2. RIKEN RESEARCH News, “Probing water molecules at cell membrane interfaces”, Dec. 28, 2017.
   https://www.riken.jp/en/news_pubs/research_news/rr/20170042/index.html
3. RIKEN RESEARCH News, “Protein changes precede photoisomerization of retinal chromophore”, Nov. 29, 2019.
   https://www.riken.jp/en/news_pubs/research_news/rr/20191129_2/index.html
4. 理研プレスリリース、“1 兆分の 3 秒で進む分子の構造変化を追跡”、2019 年 11 月 28 日.
   https://www.riken.jp/press/2019/20191128_1/index.html
   picked up by Nature Review Chemistry, **4**, 64 (2020), “Real-time bond formation”.
5. RIKEN RESEARCH News, “Gold bond formation tracked in real time using new molecular spectroscopy technique”, Feb. 14, 2020.
   https://www.riken.jp/en/news_pubs/research_news/rr/20200214_1/index.html

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加藤分子物性研究室

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Reizo KATO Chief Scientist RIKEN Cluster for Pioneering Research Condensed Molecular Materials Laboratory 2-1 Hirosawa Wako Saitama 351-0198 JAPAN +81-(0)48-467-9408 reizo@riken.jp 
Education	1979-1984 Graduate School of Science, The University of Tokyo 1977-1979 The University of Tokyo, Faculty of Science, Department of Chemistry 1974-1977 The University of Tokyo, College of General Education
Degrees	Dr. Sci. (1984) The University of Tokyo M. Sci. (1981) The University of Tokyo B. Sci. (1979) The University of Tokyo
Employment/research experience	1999- Chief Scientist, Condensed Molecular Materials Laboratory, RIKEN 1990-1999 Associate Professor, Institute for Solid State Physics, The University of Tokyo 1988-1990 Lecturer, Department of Chemistry, Faculty of Science, Toho University 1984-1988 Research Associate, Department of Chemistry, Faculty of Science, Toho University <u>Additional post</u> 2014- Visiting Professor, Gakushuin University 2013-2019 Visiting Professor, Waseda University 2011- Visiting Professor, Chiba University 2004-2007 Science Adviser, Ministry of Education, Culture, Sports, Science and Technology, Research Promotion Bureau 2003- Visiting Professor, Toho University 2002- Visiting Professor, Saitama University 2001-2002 Visiting Professor, Institute for Molecular Science
Awards and honors	Japan Society for Molecular Science Award (2017) American Physical Society (APS) Fellow (2015) MEXT Prizes for Science and Technology (2013) Chemical Society of Japan Award for Creative Work (2011) IBM Japan Science Prize (1995) Chemical Society of Japan Award for Young Chemists (1990)
Academic activities	Associate editor; Chemistry Letters (2010-2012) Member; Chemical Society of Japan Member; Physical Society of Japan Member; American Physical Society

	Member; Organizing Committee of International Symposium on Novel Electronic States in Molecular Conductors (1994) Vice-chairman, International Symposium on Cooperative Phenomena of Assembled Metal Complexes (2001) Member; Scientific Advisory Committee of International Symposium on Crystalline Organic Metals, Superconductors and Ferromagnets (2007, 2009, 2011, 2013, 2015, 2017, 2019) Member; Organizing Committee of International Conference on Science and Technology of Synthetic Metals 2010 (ICSM 2010) Member; Organizing Committee of International Symposium on the Jahn-Teller Effect (2012) Member; International Advisory Committee of International Conference on the Materials and Mechanisms of Superconductivity (2012, 2015) Member; Organizing Committee of International Symposium on Science Explored by Ultra Slow Muon (2013) Member; Organizing Committee of International Conference on Molecular-based Magnets (2016) Chairperson, The 12th International Symposium on Crystalline Organic Metals, Superconductors and Ferromagnets (2017)

(1) Participants

Reizo Kato（加藤 礼三）	主任研究員
Shigeki Fujiyama（藤山 茂樹）	専任研究員
Yugo Oshima（大島 勇吾）	専任研究員
Cui Hengbo （崔 亨波）	研究員
Yoshitaka Kawasugi（川椙 義高）	研究員
Takayuki Isono（磯野 貴之）	特別研究員
Takaaki Minamidate（南舘 孝亮）	特別研究員
Masashi Uebe（上辺 将士）	特別研究員
Lee Taehoon（李 泰勳）	JRA
Kim Sunghyun（金 星賢）	JRA
Satoshi Tajima（田島 聖士）	実習生
Hiroshi Yamamoto（山本 浩史）	客員主管研究員（分子科学研究所）
Naoya Tajima（田嶋 尚也）	客員主管研究員（東邦大学）
Takashi Yamamoto（山本 貴）	客員研究員（愛媛大学）
Masayuki Suda（須田 理行）	客員研究員（分子科学研究所）
Mitsushiro Nomura（野村 光城）	客員研究員（東京化成工業株式会社）
Takao Tsumuraya（圓谷 貴夫）	客員研究員（熊本大学）
Kohei Ueda（上田 康平）	客員研究員（東京理科大学）

(2) Original papers（ Research Category in [ ] ）

1. R. Kato and Y. Suzumura: “Novel Dirac Electron in Single-Component Molecular Conductor [Pd(dddt)$_2$] (dddt = 5,6-dihydro-1,4-dithiin-2,3-dithiolate)”, J. Phys. Soc. Jpn. **86**, 064705/1-7 (2017). [1]
2. T. Itou, E. Watanabe, S. Maegawa, A. Tajima, N. Tajima, K. Kubo, R. Kato, and K. Kanoda: “Slow Dynamics of Electrons at a Metal-Mott Insulator Boundary in an Organic System with Disorder”, Science Advances **3**, e1601594 (2017). [1]
3. H. Yamakawa, T. Miyamoto, T. Morimoto, T. Terashige, H. Yada, N. Kida, M. Suda, H. M. Yamamoto, R. Kato, K. Miyagawa, K. Kanoda, and H. Okamoto, “Mott Transition by an Impulsive Dielectric Breakdown”, Nature Materials, **16**, 1100-1105 (2017). [1]
4. T. Yamamoto, T. Fujimoto, T. Naito, Y. Nakazawa, M. Tamura, K. Yakushi, Y. Ikemoto, T. Moriwaki, and R. Kato: “Charge and Lattice Fluctuations in Molecule-Based Spin Liquids”, Scientific Reports **7**, 12930 (2017). [1]
5. E. Tisserond, J. N. Fuchs, M. O. Goerbig, P. Auban-Senzier, C. Meziere, P. Batail, Y. Kawasugi, M. Suda, H. M. Yamamoto, R. Kato, N. Tajima, and M. Monteverde: “Aperiodic Quantum Oscillations of Particle-Hole Asymmetric Dirac Cones”, EPL, **119**, 67001/1-5 (2017). [1]
6. S. Fujiyama and R. Kato: “Algebraic Charge Dynamics of the Quantum Spin Liquid β’-EtMe$_3$Sb [Pd(dmit)$_2$]$_2$”, Phys. Rev. B, **97**, 035131/1-5 (2018). [1]
7. Y. Shimizu and R. Kato: “Transport Anisotropy and Electron Correlations in the Layered Molecular Compounds Z[Pd(dmit)$_2$]$_2$ (Z=Me$_4$N,Et$_2$Me$_2$As,EtMe$_3$P) with Different Interlayer Coupling”, Phys. Rev. B **97**, 125107/1-7 (2018). [1]
8. K. Ueda, T. Tsumuraya, and R. Kato: “Temperature Dependence of Crystal Structures and Band Parameters in Quantum Spin Liquid β'-EtMe$_3$Sb[Pd(dmit)$_2$]$_2$ and Related Materials”, Crystals **8**(3), 8030138/1-15 (2018). [1]
9. S. Sugiura, K. Shimada, N. Tajima, Y. Nishio, T. Terashima, T. Isono, R. Kato, B. Zhou, and S. Uji: “Magnetocaloric Effect in Layered Organic Conductor λ-(BETS)$_2$FeCl$_4$”, J. Phys. Soc. Jpn. **87**, 044601/1-6 (2018). [1]
10. K. Sunami, T. Nishikawa, K. Miyagawa, S. Horiuchi, R. Kato, T. Miyamoto, H. Okamoto, and K. Kanoda: “Evidence for Solitonic Spin Excitations from a Charge-Lattice-Coupled Ferroelectric Order”, Science Advances **4**, eeau7725/1-6 (2018). [1]
11. T. Lee, Y. Oshima, H. B. Cui, and R. Kato: “Detailed X-band Studies of the π-d Molecular Conductor λ-(BETS)$_2$FeCl$_4$: Observation of Anomalous Angular Dependence of the g-value”, J. Phys. Soc. Jpn. **87**,

114702/1-8 (2018). [1]

12. A. Pustogow, M. Bories, A. Löhle, R. Rösslhuber, E. Zhukova, B. Gorshunov, S. Tomić, J. A. Schlueter, R. Hübner, T. Hiramatsu, Y. Yoshida, G. Saito, R. Kato, T.-H. Lee, V. Dobrosavljević, S. Fratini, and M. Dressel: "Quantum Spin Liquids Unveil the Genuine Mott State", Nature Materials **17**, 773-777 (2018). [1]
13. T. Tsumuraya, R. Kato, and Y. Suzumura: "Effective Hamiltonian of Topological Nodal Line Semimetal in Single-Component Molecular Conductor [Pd(dddt)$_2$] from First-Principles", J. Phys. Soc. Jpn. **87**, 113701/1-5 (2018). [1]
14. A. Pustogow, Y. Saito, E. Zhukova, B. Gorshunov, R. Kato, T. -H. Lee, S. Fratini, V. Dobrosavljevi, and M. Dressel: "Low-Energy Excitations in Quantum Spin Liquids Identified by Optical Spectroscopy", Phys. Rev. B **121**, 056402/1-6 (2018). [1]
15. Y. Suzumura, H. B. Cui, and R. Kato: "Conductivity and Resistivity of Dirac Electrons in Single-Component Molecular Conductor [Pd(dddt)$_2$]", J. Phys. Soc. Jpn. 87, 084702/1-6 (2018). [1]
16. R. Yamamoto, Y. Yanagita, T. Namaizawa, S. Komuro, T. Furukawa, T. Itou, and R. Kato: "Dimensionality of Superconductivity in the Layered Organic Material EtMe$_3$P[Pd(dmit)$_2$]$_2$ under Pressure", Phys. Rev. B **97**, 224502/1-5 (2018). [1]
17. W. Li, A. Pustogow, R. Kato, and M. Dressel: "Transition of a Pristine Mott Insulator to a Correlated Fermi Liquid: Pressure-Dependent Optical Investigations of a Quantum Spin Liquid", Phys. Rev. B **99**, 115137/1-8 (2019). [1]
18. P. Bourgeois-Hope, F. Laliberte, E. Lefrancois, G. Grissonnanche, S. Rene de Cotret, R. Gordon, S. Kitou, H. Sawa, H. Cui, R. Kato, L. Taillefer, and N. Doiron-Leyraud: "Thermal Conductivity of the Quantum Spin Liquid Candidate EtMe$_3$Sb[Pd(dmit)$_2$]$_2$: No Evidence of Mobile Gapless", Phys. Rev. X 9, 041051/1-8 (2019). [1]
19. J. M. Ni, B.L. Pan, B.Q. Song, Y.Y. Huang, J.Y. Zeng, Y.J. Yu, E.J. Cheng, L.S. Wang, D.Z. Dai, R. Kato, and S.Y. Li: "Absence of Magnetic Thermal Conductivity in the Quantum Spin Liquid Candidate EtMe$_3$Sb[Pd(dmit)$_2$]$_2$", Phys. Rev. Lett. 123, 247204/1-6 (2019). [1]
20. S. A. Sahadevan, A. Abherve, N. Monni, P. Auban-Senzier, J. Cano, F. Lloret, M. Julve, H. Cui, R. Kato, E. Canadell, M. L. Mercuri, and N. Avarvari: "Magnetic Molecular Conductors Based on Bis(ethylenedithio)tetrathiafulvalene (BEDT-TTF) and the Tris(chlorocyananilato)ferrate(III) Complex", Inorg. Chem., **58**, 15359-15370 (2019). [1]
21. R. Takehara, K. Sunami, K. Miyagawa, T. Miyamoto, H. Okamoto, S. Horiuchi, R. Kato, and K. Kanoda: "Topological charge transport by mobile dielectric-ferroelectric domain walls", Science Advances, 5, eaax8720/1-7 (2019). [1]
22. Y. Suzumura, T. Tsumuraya, R. Kato, H. Matsuura, and M. Ogata: "Role of Velocity Field and Principal Axis of Tilted Dirac Cones in Effective Hamiltonian of Non-Coplanar Nodal Loop", J. Phys. Soc. Jpn., **88**, 124704/1-8 (2019). [1]
23. Y. Kawasugi, K. Seki, J. Pu, T. Takenobu, S. Yunoki, H.M. Yamamoto, and R. Kato: "Non-Fermi-liquid behavior and doping asymmetry in an organic Mott insulator interface", Phys. Rev. B **100**, 115141/1-7 (2019). [5, 1]
24. Y. Kawasugi, K. Seki, S. Tajima, J. Pu, T. Takenobu, S. Yunoki, H.M. Yamamoto, and R. Kato: "Two-dimensional ground-state mapping of a Mott-Hubbard system in a flexible field-effect device", Science Advances, **5**, eaav7282/1-9 (2019). [5, 1]
25. H. Cui, T. Tsumuraya, H.H.-M. Yeung , C.S. Coates , M.R. Warren, and R. Kato: "High Pressure Crystal Structure and Electrical Properties of a Single Component Molecular Crystal [Ni(dddt)$_2$] (dddt = 5,6-dihydro-1,4-dithiin-2,3-dithiolate)", Molecules, **24**, 1843/1-12 (2019). [1]
26. S. Fujiyama and R. Kato: "Fragmented Electronic Spins with Quantum Fluctuations in Organic Mott Insulators Near a Quantum Spin Liquid", Phys. Rev. Lett. **122**, 147204/1-6 (2019). [1]
27. Y. Kiyota, T. Kawamoto, R. Kato, and T. Mori, "Thermoelectric Power of the Multi-Orbital Dimer Mott System, β-(CH$_3$)$_4$N[Pd(dmit)$_2$]$_2$", J. Phys. Soc. Jpn., **89**, 034701/1-5 (2020). [1]
28. R. Kato and Y. Suzumura, "A Tight-binding Model of an Ambient-pressure Molecular Dirac Electron System with Open Nodal Lines", J. Phys. Soc. Jpn., **89**, 044713/1-5 (2020). [1]

(3) Reviews and books （ Research Category in [ ] ）

N/A

(4) Invited presentations（ Research Category in [ ] ）

1. R. Kato: "Recent Advances in the Molecular π Electron System", RIKEN Symposium & Joint Workshop between RIKEN Nishina Center and USM, Penang, Malaysia, August (2017). [1]
2. S. Fujiyama and R. Kato: "Low Temperature Magnetic Continuum Excitation in Spin-Orbit Entangled (Cation)[Pt(dmit)$_2$]$_2$", RIKEN Symposium & Joint Workshop between RIKEN Nishina Center and USM, Penang, Malaysia, August (2017). [1]
3. Y. Oshima, S. Kim, T. Lee, and R. Kato: "Multi-Frequency ESR Studies of Molecular Magnets: Application to π-d Electrons System and Spin-Liquid System", RIKEN Symposium & Joint Workshop between RIKEN Nishina Center and USM, Penang, Malaysia, August (2017). [1]
4. H. Cui, T. Tsumuraya, and R. Kato: "Electrical Properties of Single-Component Molecular Conductors under High Pressure", 12th International Symposium on Crystalline Organic Metals, Superconductors and Magnets (ISCOM2017), Miyagi, Japan, September (2017). [1]
5. Y. Kawasugi: "Electron-Hole Doping Asymmetry in an Organic Mott Insulator Investigated by Electric-double-Layer Doping", 12th International Symposium on Crystalline Organic Metals, Superconductors and Magnets (ISCOM2017), Miyagi, Japan, September (2017). [5, 1]
6. 加藤礼三: "金属錯体 Pd(dmit)$_2$ 系の量子スピン液体相と周辺電子相"、東北大学金属材料研究所共同利用・共同研究ワークショップ　多自由度・多階層性が協奏する物質材料システムの科学、宮城県仙台市、2017 年 12 月. [1]
7. 磯野貴之: "スピン液体的振舞を示す三角格子有機磁性体の磁気特性の系統的研究", 日本物理学会第 73 回年次大会, 野田市, 2018 年 3 月. [1]
8. R. Kato: "Crystal Structure and Band Parameters of Molecular Quantum Spin Liquid and Related Materials", Seminar at the Inorganic Chemistry Laboratory, Oxford University, Oxford, UK, May (2018). [1]
9. R. Kato: "Development of Single Component Molecular Conductors", ICSM2018, Busan, South Korea, July (2018). [1]
10. Y. Kawasugi, K. Seki, S. Tajima, J. Pu, T. Takenobu, S. Yunoki, H. M. Yamamoto, and R. Kato: "Electron-Hole Doping Asymmetry of Superconductivity in a Strain-Tuned Organic Mott Transistor", Conductivity and Magnetism in Molecular Materials, Gordon Research Seminar, Charge and Spin on Molecules: Tunable Interactions and Potential Applications, Smithfield, RI, USA, August (2018). [5, 1]
11. R. Kato: "A Nodal Line Semimetal State in a Single-Component Molecular Crystal", Conductivity and Magnetism in Molecular Materials, Gordon Research Conference, Emergent Materials and Phenomena as Foundation for Future Molecule-Based Devices, Smithfield, RI, USA, August (2018). [1]
12. 川椙義高: "有機強相関トランジスタにおける両極性超伝導", 日本物理学会 2018 年秋季大会, 京田辺市, 2018 年 9 月. [5, 1]
13. R. Kato: "Single Component Molecular Conductors Based on Metal Dithiolene Complexes", The 8th Toyota RIKEN International Workshop on Organic Semiconductors, Conductors, and Electronics, 長久手市, October (2018). [1]
14. 加藤礼三: "単一成分分子性結晶の高圧下電子物性", 日本結晶学会 2018 年度年会, 東京都目黒区, November (2018). [1]
15. Y. Kawasugi: "Electron-Hole Doping Asymmetry of Superconductivity in a Strain-Tuned Organic Mott Transistor", American Physical Society March Meeting 2019, Boston, MA, USA, March (2019). [5, 1]
16. R. Kato: "Multi-Orbital Molecular Conductors Based on Metal Dithiolene Complexes", The13thInternationalSymposiumonCrystallineOrganicMetals,SuperconductorsandMagnets, Tomar, Portugal, September (2019). [1]
17. R. Kato: "A nodal line semimetal state in a single-component molecular crystal", Superstripes 2019, Ischia, Italy, June (2019). [1]

(5) Patent applications（ Research Category in [ ] ）

N/A

(6) Collaborations including both inside and outside project（ Research Category in [ ] ）

1. 加藤 礼三、圓谷貴夫（熊本大学）：分子性導体の第一原理バンド計算 [1]
2. 加藤 礼三、鈴村順三（名古屋大学）：単一成分分子性導体におけるディラック電子系に関する理論研究 [1]
3. 加藤 礼三、山本 浩史（分子研）、田嶋 尚也（東邦大）：分子性ディラック電子系の輸送現象 [1]
4. 加藤 礼三、崔 亨波、Hamish H.-M. Yeung（University of Oxford）：高圧下における単一成分分子性導体の単結晶構造解析 [1]
5. 加藤 礼三、崔 亨波、Narcis Avarvari（University of Angers）：高圧下における単一成分分子性導体の電気抵抗測定 [1]
6. 加藤 礼三、崔 亨波、圓谷貴夫（熊本大学）、Marc Fourmigué、Dominique Lorcy（Univ. Rennes, CNRS, ISCR）：単一成分分子性導体の電子構造および高圧下電気抵抗 [1]
7. 加藤 礼三、山本 貴（愛媛大学）：分子性量子スピン液体および関連物質の振動分光 [1]
8. 加藤 礼三、L. Taillefer（Université de Sherbrooke）：分子性量子スピン液体の熱伝導率 [1]
9. 加藤 礼三、S.Y. Li（Fudan University）：分子性量子スピン液体の熱伝導率 [1]
10. 加藤 礼三、松田 祐司（京都大）、山下 穣（東大）：分子性量子スピン液体の熱伝導率 [1]
11. 加藤 礼三、澤 博（名古屋大）：放射光X線を用いた、分子性量子スピン液体の構造研究 [1]
12 加藤 礼三、Martin Dressel（Universität Stuttgart）：分子性量子スピン液体の光学スペクトル [1]
13. 加藤 礼三、渡邊功雄（岩崎中間子科学研究室）、岩崎雅彦（岩崎中間子科学研究室）：分子性量子スピン液体のμSR [1]
14. 加藤 礼三、上田 康平（東京理科大）：分子性量子スピン液体の低温結晶構造 [1]
15. 加藤 礼三、伊藤 哲明（東京理科大）：分子性量子スピン液体および関連物質の NMR [1]
16. 加藤 礼三、川椙 義高、山本 浩史（分子研）、須田 理行（分子研）：有機モット系における電界/歪み制御による電子相の研究 [5, 1]
17. 加藤 礼三、川椙 義高、山本 浩史（分子研）、柚木 清司（柚木計算物性物理研究室）：有機モット系における反強磁性および d 波超伝導の秩序変数の計算 [5, 1]
18. 加藤 礼三、上野 秀樹（上野核分光研究室）：ダイヤモンドのドーピングによる超伝導探索 [3]

(7) Hosted seminars and symposiums

1. "The 12th International Symposium on Crystalline Organic Metals, Superconductors and Magnets (ISCOM2017), Miyagi, Japan, September 24-29 (2017).
2. 「物質階層原理研究」第 1 回春期研究会、御殿場市、2017 年 5 月 12-13 日.
3. 「物質階層原理研究」2017 年度研究報告会, 和光市, 2018 年 2 月 13-14 日.
4. Symposium "S21 Recent advances in molecular conductors: functionality" in 43rd International Conference on Coordination Chemistry (ICCC2018), Miyagi, Japan, July 30 – August 4 (2018).
5. 「物質階層原理研究」&「ヘテロ界面研究」2018 年度研究報告会, 和光市, 2019 年 2 月 5-6 日.

(8) Awards and honors

1. 加藤 礼三："第 8 回分子科学会賞"、分子科学会、2017 年 9 月 15 日.
2. 磯野 貴之："日本物理学会若手奨励賞"、日本物理学会、2017 年 10 月.
3. 南舘 孝亮："ISCOM2019 Poster Award"、ISCOM2019、2019 年 9 月.

(9) Press releases

1. 科学新聞、"金属状態と絶縁状態との間でゆっくりと行き来する電子"、2017 年 9 月 1 日.
2. 愛媛大学、理化学研究所、公益財団法人高輝度光科学研究センター共同プレスリリース、"分子結晶におけるスピン液体の起源を解明"、2017 年 10 月 11 日.
   https://www.ehime-u.ac.jp/wp-content/uploads/2017/10/67f414dde7cb509ee29d31a57463d2ad.pdf
3. 科学新聞、"結晶中の分子が集団変形「スピン液体」起源解明"、2017 年 10 月 27 日.
4. 理研ニュース（研究最前線）"π電子が示す多様な物性を探究する　量子スピン液体と質量のないディラック電子の新展開"、2017 年 12 月 7 日.
   https://www.riken.jp/medialibrary/riken/pr/publications/news/2017/rn201712.pdf
5. YouTube 理研チャンネル、"60 秒でわかる？π電子が示す多様な物性を探求する"、2017 年 12 月 7 日.

https://www.youtube.com/watch?v=eiQ3dV6V_Ic
6. 理研プレスリリース、“強誘電体から発現するトポロジカルなスピン励起－電荷と格子が強く結合した場を動き回るスピンソリトン－”、2018 年 12 月 4 日.
https://www.riken.jp/press/2018/20181204_1/
7. 理研プレスリリース、“分裂する量子スピン－分子内で電子の内部自由度が誘起された新スピン秩序を発見－”、2019 年 4 月 12 日.
https://www.riken.jp/press/2019/20190413_1/
8. 科学新聞、“分子内で電子内部自由度が誘起”、2019 年 5 月 10 日.
9. 理研プレスリリース、“有機トランジスタで超伝導の条件を探る－電圧とひずみで試料の超伝導を制御－”、2019 年 5 月 11 日.
https://www.riken.jp/press/2019/20190511_1/
10. 電波新聞、“有機トランジスタで超伝導の条件を探る-電圧とひずみで試料の超伝導を制御-”、2019 年 5 月 11 日.
11. 東京大学・理研プレスリリース、“トポロジカル励起による新たな電気伝導機構の解明－電荷を持ったドメインウォールの輸送現象－”、2019 年 11 月 18 日.
https://www.riken.jp/press/2019/20191118_3/index.html

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Mizuo MAEDA Chief Scientist RIKEN Cluster for Pioneering Research Bioengineering Laboratory 2-1 Hirosawa Wako Saitama 351-0198 JAPAN +81-(0)48-467-9312 mizuo@riken.jp 
Education	1978-1983 The University of Tokyo, Graduate School of Engineering, Department of Synthetic Chemistry 1976-1978 The University of Tokyo, Faculty of Engineering, Department of Synthetic Chemistry 1974-1976 The University of Tokyo, College of Liberal Arts
Degrees	Dr. Eng. from Department of Synthetic Chemistry, The University of Tokyo, Japan (1983) M.S. from Department of Synthetic Chemistry, The University of Tokyo, Japan (1980) B.S. from Department of Synthetic Chemistry, The University of Tokyo, Japan (1978)
Employment/research experience	2001-present: Chief Scientist, RIKEN 1995-2002: Professor, Kyushu University 1988-1995: Associate Professor, Kyushu University 1983-1988: Assistant Professor, The University of Tokyo <u>Additional post</u> 2016-present: Professor, Shinshu University (cross appointment with RIKEN) 2006-present: Adjunct Professor, The University of Tokyo 2004: Invited Professor, University of Louis Pastuer, France 2004-2017: Visiting Professor, Tokyo University of Science 2002-present: Visiting Professor, Kyushu University
Awards and honors	2014: Society Award (The Japan Society for Analytical Chemistry) 2011: Society Award (The Japanese Society for Biomaterials) 2009: Award for Creative Work (The Chemical Society of Japan) 2007: Commendation for Science and Technology by the MEXT (MEXT, Japan) 2005: Society Award (The Society of Polymer Science, Japan)
Academic activities	2020-present: Vice President, The Society of Polymer Science, Japan. 2018-present: Scientific Adviser to Precision System Science Co., Ltd. 2016-present: Chair, Selection and Evaluation Committee of MEXT diversity initiative program. 2016-2019: Auditor, The Japanese Society of Biomaterials. 2016-2017: Chair, RIKEN Science Council.

	2015-present: Adviser, Tohoku University committee for promotion of diversity in scientific community. 2015-2017: Auditor, The Japan Society for Analytical Chemistry. 2013-2015: Vice President, The Japan Society for Analytical Chemistry. 2011: Member, Nomination committee, Kyoto Prize. 2008-present: Fellow, International Union of Biomaterials Science and Engineering. 2008-2013: Head Investigator, MEXT Grand-in-Aid for Scientific Research on Innovative Areas, "Molecular Science of Soft Interfaces", which consisted of 52 research groups from Japanese universities and national research institutes, showing that the Chief Scientist has been well recognized as a top leader in the field of molecular interface science in Japan. 2005-present: Member, Screening Committee, Ichimura Foundation for New Technology.

(1) Participants

Mizuo Maeda（前田 瑞夫）	主任研究員
Kazunari Ozasa（尾笹 一成）	専任研究員
Tohru Takarada（宝田 徹）	専任研究員
Masahiro Fujita（藤田 雅弘）	専任研究員
Young-Jin Kim（金 栄鎮）	基礎科学特別研究員
Rodtichoti Wannapob	特別研究員
Yuji Tsuchido（土戸 優志）	協力研究員
Chia-Chen Chang（張 家禎）	訪問研究員
Takafumi Sako（佐孝 貴文）	JRA
Li Yu（余 力）	IPA
Surachada Chuaychob	IPA
Tzung-Ying Yang（楊 宗穎）	研修生
Yoshifumi Sakamoto（坂本 佳史）	研修生
Michitsuna Tsutsumi（堤 未智綱）	研修生
Naoki Kanayama（金山 直樹）	客員研究員（信州大学）
Yoshitsugu Akityama（秋山 好嗣）	客員研究員（東京理科大学）
Guoqing Wang（王 国慶）	客員研究員（中国海洋大学）

(2) Original papers（Research Category in [ ]）

1. G. Wang, T. Bu, T. Zako, R. Watanabe-Tamaki, T. Tanaka, and M. Maeda: "Dark Field Microscopic Analysis of Discrete Au Nanostructures: Understanding the Correlation of Scattering with Stoichiometry", Chem. Phys. Lett. **684**, 310-315 (2017). [1]
2. C. C. Chang, G. Wang, T. Takarada, and M. Maeda: "Iodine-Mediated Etching of Triangular Gold Nanoplates for Colorimetric Sensing of Copper Ion and Aptasensing of Chloramphenicol", ACS Appl. Mater. Interfaces **9**, 34518-34525 (2017). [1]
3. G. Wang, Y. Liu, C. Gao, K. Ijiro, M. Maeda, and Y. Yin: "Island Growth in the Seed-Mediated Overgrowth of Monometallic Colloidal Nanostructures", Chem **3**, 678-690 (2017). [1]
4. G. Wang, Y. Akiyama, N. Kanayama, T. Takarada, and M. Maeda: "Directed Assembly of Gold Nanorods by Terminal-Base Pairing of Surface-Grafted DNA", Small **13**, 1702137/1-8 (2017). [1]
5. S. Shiraishi, L. Yu, Y. Akiyama, G. Wang, T. Kikitsu, K. Miyamura, T. Takarada, and M. Maeda: "Folding of Nanoparticle Chains into 2D Arrays: Structural Change of DNA-Functionalized Gold Nanoparticle Assemblies", Adv. Mater. Interfaces **5**, 1800189/1-7 (2018). [1]
6. K. Ozasa, J. Won, S. Song, and M. Maeda: "Bio-Inspired Neurocomputing with 256 Noise Oscillators Simulating Photo Response of *Euglena* Cells", Appl. Soft Comput. **70**, 539–549 (2018). [1]
7. K. Ozasa, J. Won, S. Song, and M. Maeda: "Behavior of *Euglena Gracilis* under Simultaneous Competing Optical and Chemical Stimuli", Algal Res. **35**, 98–105 (2018). [1]
8. Z. L. Tang, T. Takarada, and M. Maeda: "Non-Cross-Linking Aggregation of DNA-Carrying Polymer Micelles Triggered by Duplex Formation", Langmuir **34**, 14899–14910 (2018). [1,4]
9. T. Sekine, N. Kanayama, K. Ozasa, T. Nyu, T. Hayashi, and M. Maeda: "Stochastic Binding Process of Blunt-End Stacking of DNA Molecules Observed by Atomic Force Microscopy", Langmuir **34**, 15078–15083 (2018). [1]
10. G. Wang, L. Yu, Y. Akiyama, T. Takarada, and M. Maeda: "Reversible Shrinkage of DNA-Functionalized Gold Nanoparticle Assemblies Revealed by Surface Plasmon Resonance", Biotechnol. J. **13**, 1800090/1-4 (2018). [1]
11. C. Zhao, G. Wang, T. Takarada, X. Liang, M. Komiyama, and M. Maeda: "Shape-Selective Isolation of Au Nanoplates from Complex Colloidal Media by Depletion Flocculation", Colloids Surf. A **568**, 216–223 (2019). [1]
12. C. C. Chang, G. Wang, T. Takarada, and M. Maeda: "Target-Recycling-Amplified Colorimetric Detection of Pollen Allergen Using Non-Cross-Linking Aggregation of DNA-Modified Gold

Nanoparticles", ACS Sens., **4**, 363-369 (2019). [4]

13. G. Wang, Y. Zhang, X. Liang, T. Takarada, and M. Maeda: "Regioselective DNA-Modification and Directed Self-Assembly of Triangular Gold Nanoplates", Nanomaterials **9**, 581/1–8 (2019). [1]
14. L. Yu, S. Shiraishi, G. Wang, Y. Akiyama, T. Takarada, and M. Maeda: "Connecting Nanoparticles with Different Colloidal Stability by DNA for Programmed Anisotropic Self-Assembly", J. Phys. Chem. C **123**, 15293–15300 (2019). [1]
15. L. Zhang, C. Zhao, Y. Zhang, L. Wang, G. Wang, N. Kanayama, T. Takarada, M. Maeda, and X. Liang: "Chemically Fueled Plasmon Switching of Gold Nanorods by Single-Base Pairing of Surface-Grafted DNA", Langmuir **35**, 11710–11716 (2019). [4]
16. F. Ito, M. Saigusa, and N. Kanayama: "Evaporative Crystallization of Dibenzoylmethanato Boron Difluoride Probed by Time-Resolved Quartz Crystal Microbalance Responses with Fluorescence Changes", Chem. Lett. **48**, 1199–1202 (2019). [1]
17. Y. Yano, M. Nisougi, Y. Yano-Ozawa, T. Ohguni, A. Ogawa, M. Maeda, T. Asahi, and T. Zako: "Detection of Gold Nanoparticles Aggregation Using Light Scattering for Molecular Sensing", Anal. Sci. **35**, 685–690 (2019). [4]
18. K. Sato, K. Hosokawa, and M. Maeda: "Characterizing the Non-Crosslinked Aggregation of DNA-Modified Gold Nanoparticles: Effects of DNA Length and Terminal Base Pair", Analyst **144**, 5580–5588 (2019). [4, 1]
19. K. Ozasa, J. Won, S. Song, T. Shinomura, and M. Maeda: "Phototaxis and Photo-Shock Responses of *Euglena Gracilis* under Gravitaxis", Algal Res. **41**, 101563 (2019). [1]
20. Y.-J. Kim, K. Hosokawa, and M. Maeda: "Sensitivity Enhancement of MicroRNA Detection Using a Power-Free Microfluidic Chip", Anal. Sci. **35**, 1227–1236 (2019). [4]
21. S. Chuaychob, C. Thammakhet-Buranachai, P. Kanatharana, P. Thavarungkul, C. Buranachai, M. Fujita, and M. Maeda: "A Nanobiosensor for the Simple Detection of Small Molecules Using Non-Crosslinking Aggregation of Gold Nanoparticles with G-Quadruplexes", Anal. Methods **12**, 230–238 (2020). [4, 1]
22. S. Kato, K. Ozasa, M. Maeda, Y. Tanno, S. Tamaki, M. Higuchi-Takeuchi, K. Numata, Y. Kodama, M. Sato, K. Toyooka, and T. Shinomura: "Carotenoids Are Essential for Light Perception by the Eyespot Apparatus to Initiate the Phototactic Movement of *Euglena Gracilis*", Plant J. **101**, 1091-1102 (2020). [1]
23. L. Wang, G. Wang, Y. Shi, L. Zhang, R. An, T. Takarada, M. Maeda, and X. Liang: "Accelerated Non-Crosslinking Assembly of DNA-Functionalized Nanoparticles in Alcoholic Solvents: Towards Application in Identification of Clear Liquors", Analyst, in press. [4]

(3) Reviews and books（ Research Category in [ ] ）

1. 宝田徹、前田瑞夫："ナノ粒子による精密診断"、CSJ カレントレビュー24　医療・診断・創薬の化学、日本化学会編、化学同人、**24**、63-69 (2017). [1]
2. 金山直樹："「見て診る」ための金ナノ粒子"～小さな金の大きなチカラ～、ファルマシア、**54(1)**、3135 (2018). [1]
3. 藤田雅弘、前田瑞夫："第２編　第１章　温度応答性　第３節　温度応答性高分子と DNA との複合化と認識挙動"、宮田隆志　監修「刺激応答性高分子ハンドブック」、2018 年 12 月刊行. [4,1]
4. G. Wang, Y. Akiyama, N. Kanayama, T. Takarada, and M. Maeda: "Non-Crosslinking Aggregation of DNA-Functionalized Gold Nanoparticles for Gene Diagnosis and Directed Assembly", ACS Symposium Series "Targeted Nanosystems for Therapeutic Applications: New Concepts, Dynamic Properties, Efficiency & Toxicity", Edited by M. Ilies and K. Sakurai, Oxford University Press, **1309**, 119-138 (2019). [1,4]
5. M. Maeda, A. Takahara, H. Kitano, T. Yamaoka, and Y. Miura (Eds): "Molecular Soft-Interface Science: Principles, Molecular Design, Characterization and Application", Springer Japan (2019). [1, 4]
6. 前田瑞夫："DNA 超分子の化学 –精密遺伝子診断・DNA 工学への展開–"、現代化学、2020 年 1 月号、No. 586、48–50 (2020). [4]
7. 金山直樹、前田瑞夫："DNA 修飾金ナノ粒子の特性を活かした精密遺伝子診断法"、核酸科学ハンドブック、日本核酸化学会 監修（杉本直己編集）、講談社サイエンティフィク、印刷中. [4]

(4) Invited presentations（ Research Category in [ ] ）

1. M. Maeda: “Non-Cross-Linking Aggregation of Nanoparticles Carrying Double-Stranded DNA: Directed Assembly, Mechanism, and Sensor Application”, The 2017 International Advanced Drug Delivery Symposium (IADDS), Taipei, Taiwan, Apr. (2017). [1]
2. 藤田雅弘、前田瑞夫：“DNA 担持ナノ粒子の物性とそれを活かした検出機能”、第 77 回分析化学討論会、京都府京都市、2017 年 5 月．[4]
3. 宝田徹：“DNA 複合高分子を用いたアフィニティー分離システムによる遺伝子分析”、第 77 回分析化学討論会、京都府京都市、2017 年 5 月．[4]
4. 前田瑞夫：“DNA 二重らせん担持ナノ粒子を用いる精密バイオセンシング”、生物化学的測定研究会 第 22 回学術集会プログラム、東京都、2017 年 6 月．[4]
5. 前田瑞夫：“DNA–合成高分子複合体（DNA コンジュゲート）の合成と診断応用”、香川大学 アドバンスト・セミナー、香川県高松市、2017 年 6 月．[1]
6. 前田瑞夫：“DNA コンジュゲート材料の開発と展開”、2017 年バイオ工学シンポジウム、愛媛県松山市、2017 年 7 月．[1]
7. 前田瑞夫：“DNA 二重鎖がつくるソフトな界面の特異な性質とその応用”、平成 29 年度生理研研究会、愛知県岡崎市、2017 年 7 月．[1]
8. M. Fujita, M. Maeda: “Non-crosslinking Aggregation of DNA-functionalized Gold Nanoparticles”, The 15th International Conference on Advanced Materials (IUMRS-ICAM 2017), Kyoto, Aug.-Sep. (2017). [1]
9. M. Maeda: “Nano-Bio Architectures from Double-Stranded DNA-Functionalized Nanoparticles”, Advanced Materials for Biomedical Applications (AMBA 2017), Ghent, Belgium, Sep. (2017). [1]
10. 宝田徹：“高分子プローブの流体抵抗に基づく DNA の電気泳動分離”、日本分析化学会第 66 年会、東京都、2017 年 9 月．[4]
11. 宝田徹：“DNA 修飾ナノ粒子集合体の特異な異方構造形成：分析化学への適用可能性”、日本分析化学会第 66 年会、東京都、2017 年 9 月．[1]
12. 前田瑞夫：“ソフトな界面の研究、過去現在未来”、第 27 回日本 MRS 年次大会、神奈川県横浜市、2017 年 12 月．[1]
13. G. Wang: “Spontaneous Aggregation of DNA-modified Anisotropic Gold Nanoparticles for Gene Diagnosis and Directed Assembly”, The 15th Pacific Polymer Conference (PPC-15), Xiamen, China, Dec. (2017). [1]
14. 宝田徹：“キャピラリー電気泳動を用いる遺伝子変異検出”、第 2 回信大・理研ソフトマター交流サロン、長野県長野市、2017 年 12 月．[4]
15. C. C. Chang: “Gold Nanoparticle-Based Colorimetric Strategies for Biosensing Applications”、第 2 回信大・理研ソフトマター交流サロン、長野県長野市、2017 年 12 月．[4]
16. G. Wang: “Island Growth in the Seeded Overgrowth of Colloidal Gold Nanostructures”、第 3 回信大・理研ソフトマター交流サロン、長野県長野市、2018 年 1 月．[1]
17. M. Maeda: “Nano-Bio Sensing Systems Using Double-Stranded DNA-Functionalized Nanoparticles”, Pure and Applied Chemistry International Conference (PACCON 2018), Hat Yai, Thailand, Feb. (2018). [4]
18. 前田瑞夫: “核酸二重鎖担持コロイドで分析する”、第 78 回分析化学討論会、宇部市、2018 年 5 月. [4]
19. K. Ozasa: “Microalgae Cells in Microfluidic Devices”, 2018 Hanyang INST Symposium "Functional Nanomaterials and Systems", Seoul, South Korea, Jun. (2018). [1]
20. 宝田徹: “Non-Crosslinking Aggregation of DNA-Functionalized Nanoparticles for Gene Diagnosis and Directed Assembly”、平成 30 年度化学系学協会東北大会、秋田市、2018 年 9 月. [1]
21. 土戸 優志:”Development of functional nanoparticles for the detection of bacteria“、2018 Fall Meeting of The Korean Society for Biomaterials、韓国城南市、2018 年 10 月. [1]
22. 宝田徹: “コロイドを DNA でつなぐ：等方的なナノ粒子の異方的な自己集合”、信州コロイド＆界面科学研究センター第 4 回研究討論会、長野市、2018 年 10 月. [1]
23. 前田瑞夫: “DNA 二重鎖の界面集積化がもたらす新機能”、第 49 回中化連特別討論会、名古屋市、2018 年 11 月. [4]

24. M. Maeda: “Small DNA Molecule as Unique Surface-Modifier Capable of Controlling Material Surface Interaction”, The 19th RIES-Hokudai International Symposium, Sapporo, Dec. (2018). [1]
25. R. Wannapob: “Development of Electrochemical Sensors and Biosensors based on Porous Electrode and Conducting Polymer”、国立大学法人九州工業大学 第 61 回歯工学連携講演会、福岡県北九州市、2019 年 8 月. [4]
26. 金山直樹: “部位特異的な DNA 鎖間のチカラをはかる ～ナノ・ピコ力学計測への挑戦”、第 50 回 中部化学関係学協会支部連合秋季大会 特別討論会「新時代を開拓する分析化学」、長野県松本市、2019 年 11 月. [1]
27. 金山直樹: “スマートな色材を指向した DNA 修飾プラズモンナノ粒子”、第 50 回 中部化学関係学協会支部連合秋季大会 特別討論会「コロイドが彩る色材の世界」、長野県松本市、2019 年 11 月. [4]
28. 尾笹一成:“ユーグレナの定量的運動解析とその応用－運動観察からのトップダウンアプローチ－”、ユーグレナ研究会第３５回研究集会、大阪市、2019 年 11 月. [1]
29. M. Maeda: “Double-Stranded DNA-Carrying Nanoparticles for Chemical and Biomedical Sensing”, 16th Pacific Polymer Conference, Suntec City, Singapore, Dec. (2019). [4]
30. M. Maeda: “DNA Conjugates for Reliable Genotyping”, Trace Analysis and Biosensor International Symposium I, Hat Yai, Thailand, Feb. (2020). [4]
31. S. Chuaychob: “Colorimetric Thrombin Sensor using DNA Aptamer-modified Gold Nanoparticles”、日本化学会 第 100 春季年会、千葉県野田市、2020 年 3 月 [4]

(5) Patent applications（ Research Category in [ ] ）

N/A

(6) Collaborations including both inside and outside project（ Research Category in [ ] ）

1. 前田瑞夫、王国慶、居城邦治（北海道大学）: 金ナノ材料の構造解析 [1]
2. 前田瑞夫、王国慶、Yadong Yin（University of California, Riverside）: 金ナノ材料の合成 [1]
3. 前田瑞夫、宝田徹、宮村一夫（東京理科大学）: ナノ粒子集合体の構造解析 [1]
4. 前田瑞夫、宝田徹、唐中嵐（四川大学）: 高分子ミセルの機能評価 [1, 4]
5. 前田瑞夫、宝田徹、梁興国（中国海洋大学）: DNA の熱力学的安定性の理論予測 [1]
6. 前田瑞夫、座古保（愛媛大学）: ナノ粒子集合体の構造解析 [4]
7. 前田瑞夫、小川敦司（愛媛大学）: 機能性核酸の分子設計 [4]
8. 前田瑞夫、佐藤香枝（日本女子大学）: DNA 修飾ナノ粒子の物性評価 [4, 1]
9. 前田瑞夫、宝田徹、秋山好嗣、菊池明彦（東京理科大学）: DNA 親和性薬物の検出法 [4]

(7) Hosted seminars and symposiums

1. 「物質階層原理研究」第 1 回春期研究会、御殿場市、2017 年 5 月 12-13 日.
2. 信州コロイド＆界面科学研究センター第 4 回研究討論会「信大－理研特別セッション」、長野市、2018 年 10 月 27 日.
3. “食品 3D プリンタの開発”、武政 誠 博士（東京電機大学理工学部生命理工学系　准教授）、2019 年 11 月 21 日.
4. “Strategies of Immobilizing Cells in Whole-Cell Microbial Biosensor Devices”, Ms. Nadine Lobsiger (Department of Chemistry and Applied Biosciences, ETH Zürich, Switzerland), 2019 年 12 月 20 日.
5. 2019 年度「物質階層原理研究」＆「ヘテロ界面研究」研究報告会、和光市、2020 年 2 月 4-5 日.

(8) Awards and honors

1. G. Wang: “Excellent Poster Prize Award”, 13th IUPAC International Conference on Novel Materials and their Synthesis (NMS-XIII), Nanjing, China, October 15-20 (2017).
2. S. Chuaychob, M. Fujita, and M. Maeda:“第 40 回日本バイオマテリアル学会優秀研究ポスター賞”、

日本バイオマテリアル学会、2018 年 11 月 13 日.

3. 土戸優志：“2018 年度新世紀新人賞”、日本分析化学会関東支部、2019 年 1 月 8 日.
4. 余力：“第 68 回高分子学会年次大会 優秀ポスター賞”、高分子学会、2019 年 5 月 31 日.
5. S. Chuaychob: “RIKEN Summer School 2019 Poster Award: Chemistry Prize & Special Prize for Most Inclusive Presentation”, RIKEN, 2019 年 10 月 8 日.
6. S. Chuaychob: “Trace Analysis and Biosensor International Symposium I: Best Poster Presentation”, Center of Excellence for Trace Analysis and Biosensor, Prince of Songkla University, Thailand, 2020 年 2 月 11 日.

(9) Press releases

1. 日経産業新聞、“新たな抗がん剤候補物質 色の変化で簡単探索”、2018 年 9 月 28 日.

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Yoshitsugu Shiro Professor University of Hyogo, Graduate School of Life Science, Cellular Regulation Laboratory 3-2-1 Kouto, Kamigori, Ako-gun, Hyogo 678-1297, JAPAN +81-(0)791-58-0325 yshiro@sci.u-hyogo.ac.jp 
Education	1980-1985 Graduate School of Engineering, Kyoto University 1976-1980 Kyoto University, Faculty of Engineering, Department of Hydrocarbon Chemistry
Degrees	Dr. Eng. (1985) Kyoto University M. Eng. (1982) Kyoto University B. Eng. (1980) Kyoto University
Employment/research experience	2015- Professor, Cellular Regulation Laboratory, University of Hyogo 2000-2015 Chief Scientist, RIKEN SPring-8 Center 1993-2000 Senior Research Scientist, RIKEN 1987-1993 Research Scientist, RIKEN 1985-1987 Postdoctral Fellowship of JSPS <u>Additional post</u> 2016-2018 Visiting Professor, Institute for Materials Chemistry and Engineering, Kyusyu University 2006-2014 Professor, Joint Program of Graduate School of Science, Osaka University 2007- Professor, Joint Program of Graduate School of Science, Nagoya University 2005-2007 Professor, Joint Program of Graduate School of Science, Kyoto University 2000- Visiting Professor, Institute of Multidisciplinary Research on Advanced Materials, Tohoku University 1999-2015 Professor, Joint Program of Graduate School of Science, University of Hyogo 1991-1992 Visiting Scholar, Department of Chemistry, Stanford University, California, USA
Awards and honors	Japan Society for Coordination Chemistry, Contribution Award (2019)
Academic activities	Member; Chemical Society of Japan Member; The Japanese Biochemical Society Member; The Biophysical Society of Japan Member; Protein Science Society of Japan Local Program Committee of "The 11th International Conference on X-ray

	Absorption Fine Structure (XAFS IX)" (2000) Local Steering Committee of "The 8th International Conference on Biology and Synchrotron Radiation (BSR2004)" (2004) Chair of Program Committee of "14th International Conference on Biological Inorganic Chemistry (ICBIC14)" (2009) Board member of Protein Science Society of Japan (2009 - 14, 16-17) Organizing Committee of "16th International Conference on Cytochrome P450" (2009) Chair of Organizing Committee of "50th Anniversary Symposium on Cytochrome P450 in Fukuoka" (2012) Member of Organizing Committee of "16th International Conference on Cytochrome P450" (2014) Member of Organizing Committee of "12th International Conference on Cytochrome P450; Biodiversity & Biotechnology" (2015) Vice President of Protein Science Society of Japan (2018 - 20) Co-chair of 19th Annual Meeting of Protein Science Society of Japan (Joint Conference with Japan Society of Cell Biology) (2019) Co-chair of 11th Asian Biological Inorganic Chemistry Conference (AsBIC-11) (2022)

(1) Participants

Yoshitsugu Shiro（城　宜嗣）	教授
Kazumasa Muramoto（村本　和優）	准教授
Hitomi Sawai（澤井　仁美）	助教
Yasuhiro Koteishi （小手石泰康）	特任助教
Takashi Nomura（野村　高志）	特任助教
Yudai Nishitani（西谷　雄大）	非常勤研究員
Chai Gopalasingam	非常勤研究員
Michiyo Takahara（高原　教代）	非常勤研究員
Minoru Kubo（久保　稔）	教授（生体物質構造Ⅱ研究室）
Hiro Nakamura（中村　寛夫）	専任研究員（BDR タンパク質機能・構造研究チーム）
Tamao Hisano（久野　玉雄）	専任研究員（BDR タンパク質機能・構造研究チーム）
Hiroshi Sugimoto（杉本　宏）	専任研究員（RSC 生命系放射光利用システム開発チーム）
Takehiko Tosha（當舎　武彦）	専任研究員（RSC 生命系放射光利用システム開発チーム）

(2) Original papers（Research Category in [ ]）

1. E. Terasaka, K. Yamada, P.-H. Wang, K. Hosokawa, R. Yamagiwa, K. Matsumoto, S. Ishii, T. Mori, K. Yagi, H. Sawai, H. Arai, H. Sugimoto, Y. Sugita, Y. Shiro, T. Tosha: "Dynamics of Nitric Oxide Controlled by Protein Complex in Bacterial System" *Proc. Natl. Acad. Sci. USA* **114**, 9888-9893 (2017) [1]
2. T. Tosha, T. Nomura, T. Nishida, N. Saeki, K. Okubayashi, R. Yamagiwa, M. Sugahara, T. Nakane, K. Yamashita, K. Hirata, G. Ueno, T. Kimura, T. Hisano, K. Muramoto, H. Sawai, H. Takeda, E. Mizohata, A. Yamashita, Y. Kanematsu, Y. Takano, E. Nango, R. Tanaka, O. Nureki, Y. Ikemoto, H. Murakami, S. Owada, K. Tono, M. Yabashi, M. Yamamoto, H. Ago, S. Iwata, H. Sugimoto, Y. Shiro, M. Kubo: "Capturing an Initial Intermediate during Enzymatic Reaction of P450nor using Time-Resolved XFEL Crystallography and Caged-Substrate" *Nat. Commun.* **8**, 1585 (2017) [2]
3. Y. Naoe, N. Nakamura, Md. M. Rahman, T. Tosha, S. Nagatoishi, K. Tsumoto, Y. Shiro, H. Sugimoto: "Structural Basis for the Capture and Transfer of Heme by Periplasmic Heme-Binding Proteins in a Bacterial Heme-Acquisition System" *PROTEINS: Structure, Function and Bioinformatics* **85**, 2217-2230 (2017) [1]
4. H. Uehara, Y. Shisaka, T. Nishimura, H. Sugimoto, Y. Shiro, Y. Miyake, H. Shinokubo, Y. Watanabe, O. Shoji: "Structure of the Heme Acquisition Protein HasA with Iron(III)-5, 15-Diphenyl-Porphyrin and Derivatives Thereof as an Artificial Prosthetic Group" *Angew. Chem. Int. Ed.* **56**, 1-6 (2017) [1]
5. K. Oohora, H. Meichin, Y. Kihira, H. Sugimoto, Y. Shiro, T. Hayashi: "A Manganese(V) Porphycene Complex Responsible for Inert C–H Bond Hydroxylation in Myoglobin Matrix" *J. Am. Chem. Soc.* **139**, 18461-18463 (2017) DOI: 10.1021/jacs.7b11288 [1]
6. N. Gonska, D. R. Young, R. Yuki, T. Okamoto, T. Hisano, S. V. Antonyuk, S. S. Hasnain, K. Muramoto, Y. Shiro, T. Tosha, P. Ädelroth: "Characterization of the Quinol-dependent Nitric Oxide Reductase from the Pathogen *Neisseria meningitidis*, an Electrogenic Enzyme." *Sci. Rep.* **8**, 3637 (2018) DOI: 10.1038/s41598-018-21804-0 [4, 1]
7. R. Yamagiwa, T. Kurahashi, M. Takeda, M. Adachi, H. Nakamura, H. Arai, Y. Shiro, H. Sawai, T. Tosha: "*Pseudomonas aeruginosa* Overexpression System of Nitric Oxide Reductase for *in vivo* and *in vitro* Mutational Analyses" *Biochim. Biophys. Acta Bioenergetics* **1859**, 333-341 (2018) DOI: 10.1016/j.bbabio.2018.02.009 [4]
8. R. Makino, Y. Obata, M. Tsubaki, T. Iizuka, Y. Hamajima, Y. Kato-Yamada, K. Mashima, Y. Shiro: "Mechanistic Insights into the Activation of Soluble Guanylate Cyclase by Carbon Monoxide: A Multi-Step Mechanism Proposed for the BAY 41-2272-Induced Formation of 5-Coordinate CO–Heme" *Biochemistry* **57**, 1620–1631 (2018) DOI: 10.1021/acs.biochem.7b01240 [1]
9. G. S. A. Wright, A. Saeki, T. Hikima, Y. Nishizono, T. Hisano, M. Kamaya, K. Nukina, H. Nishitani, H. Nakamura, M. Yamamoto, S. V. Antonyuk, S. S. Hasnain, Y. Shiro, H. Sawai: "Architecture of the Complete Oxygen-Sensing FixL-FixJ Two-Component Signal Transduction System"" *Sci. Signal.* **11**, aaq0825 (2018) DOI: 10.1126/scisignal.aaq0825 [1]

10. M. Ganasen, H. Togashi, H. Takeda, H. Asakura, T. Tosha, K. Yamashita, K. Hirata, Y. Nariai, T. Urano, X. Yuan, I. Hamza, G. A. Mauk, Y. Shiro, H. Sugimoto, H. Sawai: "Structural Basis for Promotion of Duodenal Iron Absorption by Enteric Ferric Reductase with Ascorbate" *Commun. Biol.* 1: 120 (2018) DOI: 10.1038/s42003-018-0121-8 [4]
11. M. Kato, S. Nakagawa, T. Tosha, Y. Shiro, Y. Masuda, K. Nakata, I. Yagi: "Surface-Enhanced Infrared Absorption Spectroscopy of Bacterial Nitric Oxide Reductase under Electrochemical Control Using Vibrational Probe of Carbon Monoxide" *J. Phys. Chem. Lett.* **9**, 5196-5200 (2018) DOI: 10.1021/acs.jpclett.8b02581 [4, 1]
12. Y. Furukawa, C. T. Lim, T. Tosha, S. Akiyama, S. Watanabe, K. Nakagome, Y. Shiro: "Identification of a Novel Zinc-binding Protein, C1orf123, as an Interactor with a Heavy Metal-associated Domain" *PLoS One* **13**, e020435 (2018) DOI: 10.1371/journal.pone.0204355 [1]
13. S. Yanagisawa, K. Kayama, M. Hara, H. Sugimoto, Y. Shiro, T. Ogura: "UV-Raman Characterization of a Substrate Tryptophan Bound to Human Indoleamine 2,3-Dioxygenase 1" *Biophys. J.* ***117***, 706-716 (2019) [1]
14. C. Gopalasingam, G. Chiduza, T. Tosha, M. Yamamoto, Y. Shiro, S. V. Antonyuk, S. Muench, S. S. Hasnain: "Structure of Quinol-dependent Nitric Oxide Reductase *from Alcaligenes xylosoxidans* by Cryo-electron microscopy" *Sci. Adv.* ***5*** eaax1803 (2019) [4]
15. K. Tamura, H. Sugimoto, Y. Shiro, Y. Sugita: "Chemomechanical Coupling in the Transport Cycle of a Type II ABC Transporter" *J. Phys. Chem. B* ***123***, 7270-7281 (2019) [4]
16. Y. Shisaka, Y. Iwai, S. Yamada, H. Uehara, T. Tosha, H. Sugimoto, Y. Shiro, J. K. Stanfield, K. Ogawa, Y. Watanabe, O. Shoji: "Hijacking the haem acquisition system of *Pseudomonas aeruginosa* for antimicrobial delivery" *ACS Chemical Biology* ***14***,1637-1642 (2019) [1]
17. K. Yoshitani, E. Ishii, K. Taniguchi, H. Sugimoto, Y. Shiro, Y. Akiyama, A. Kato, R. Utsumi, Y. Eguchi: "Identification of an internal cavity in the PhoQ sensor domain for PhoQ activity and SafA-mediated control." *Biosci. Biotechnol. Biochem.* ***83***, 684 (2019) [1]
18. J. K. Stanfield, K. Omura, A. Matsumoto, C. Kasai, H. Sugimoto, Y. Shiro, Y. Watanabe, O. Shoji: "Crystals in minutes: instant on-site microcrystallisation of various flavours of the CYP102A1 (P450BM3) haem domain." *Angew. Chem. Int. Ed. Engl.* ***59***, 2-10 (2020) [1]
19. M. A. M. Jamali, C. C. Gopalasingam, R. M. Johnson, T. Tosha, K. Muramoto, S. P. Muench, S. V. Antonyuk, Y. Shiro, S. S. Hasnain: "Active form of quinol-dependent Nitric Oxide Reductases (qNOR) from *Neisseria meningitidis* is a dimer" *IUCr J.* (2020) *in press* [4]
20. H. Takeda, T. Kimura, T. Nomura, A. Yokota, A. Matsubayashi, S. Ishii, T. Tosha, **Y. Shiro**, M. Kubo: "Timing of NO binding and Protonation in Catalytic Reaction of Bacterial Nitric Oxide Reductase Proved by Time-Resolved Spectroscopic System" *Bull. Chem. Soc. Japan* (2020) *in press* [2]

(3) Reviews and books（Research Category in [ ]）

1. 杉本宏「バクテリアにおけるヘムの獲得と輸送の構造生物学」日本結晶学会誌 59**,** 166-173 (2017) [1]
2. H. Sawai, Y. Shiro: "Haem-based Sensors of Dioxygen" Chapter 3 of RSC Metallobiology Series No. 11, *Gas Sensing in Cells*, Edited by S. Aono, The Royal Society of Chemistry, 2017, pp. 47-83 [1]
3. 城　宜嗣："生体金属動態の構造ダイナミクス" 特集「生体内金属の動態解明とその制御：分子から細胞、臨床まで」生化学、90、pp. 263-271 (2018) （総説）[1, 2, 4]
4. 杉本宏, 城宜嗣「ヘム輸送体の立体構造と基質輸送メカニズム」生物物理 335**,** 5-8 (2018) [4, 1]
5. 佐伯茜子、澤井仁美："酸素を感知する FixL-FixJ 二成分シグナル伝達系の全体像" サイエンスシグナリングに載った日本人研究者 (Japanese Scientists in Science Signaling) pp. 12-13 (2019)（解説）[1]
6. 當舎武彦："酵素タンパク質複合体形成による効率的な細胞内連続化学反応" ディビジョン・トピックス（生体機能関連化学・バイオテク）化学と工業、2018 年 6 月号 p497（解説）[1, 4]
7. T. Tosha and Y. Shiro : "Structure and Function of Membrane-bound Bacterial Nitric Oxide Reductases" in *Dioxygen-dependent Heme Enzymes* (Royal Society of Chemistry Metallobiology Series No. 13), M. Ikeda-Saito and E. Raven Ed., 2019, p334-350（著書）[1, 2, 4]
8. T. Tosha and M. Kubo: "Observation of enzymatic reaction by time-resolved X-ray crystallography using photosensitive caged substrate" SPring-8/SACLA Research Frontiers 2018, *in press*（解説）[2]

9. H. Sawai, Y. Shiro: “Missing Piece of Two-Component Signal Transduction Systems Unveiled by SEC-SAXS” *SPring-8/SACLA Research Frontiers 2018*, Japan Synchrotron Radiation Research Institute (JASRI), 15-16, (2019) [1]
10. T. Tosha, M. Kubo: “Observation of Enzymatic Reactions by Time-resolved X-ray Crystallography Using Photosensitive Caged Substrate” *SPring-8/SACLA Research Frontiers 2018*, Japan Synchrotron Radiation Research Institute (JASRI), 28-29, (2019) [2]
11. M. Suga, A. Shimada, F. Akita, J.R. Shen. T. Tosha, H. Sugimoto: “Time-Resolved Studies of Metalloproteins Using X-ray Free Electron Laser Radiation at SACLA” *Biochim. Biophys. Acta – General Subjects,* ***1864***, 129466 (2020) [2]
12. 當舎武彦，久保稔 : “SACLA を利用した酵素反応の可視化　(Visualization of Enzymatic Reactions Using SACLA)” 生物物理 (SEIBUTSU BUTSURI), **59**, 205-207 (2019) [2]

(4) Invited presentations（Research Category in [ ] ）

1. Shiro, Y.: “Structural Basis fro Molecular Mechanism of Bacterial Nitric Oxide Reductases” *Intl. Conf. Physics of Life*, Nagoya, Mar. 25-26 (2017) [2]
2. G. S. A. Wright, A. Saeki, T. Hikima, Y. Nishizono, T. Hisano, M. Yamamoto, S. V. Antonyuk, S. S. Hasnain, Y. Shiro, H. Sawai: “Inter- and inter-molecular signal transduction mechanisms in a complete oxygen sensing system.” 第 17 回日本蛋白質科学会年会 ワークショップ “Protein Science in Oxygen Sensing”、2017 年 6 月 20 日、仙台 [1]
3. 杉本宏「結晶構造から明らかになった病原菌ヘムトランスポーターの分子メカニズム」第１７回日本蛋白質科学会年会ワークショップ：生体内の金属動態：Structural Dynamics of Metals in Biology、2017 年 6 月 22 日、仙台 [1]
4. 中村寛夫「ヘムは栄養であるが、毒でもある：ヘムを解毒する病原菌のヘム排出ポンプの機能と構造」第１２回トランスポーター研究会、2107 年 7 月 8-9 日、仙台 [1]
5. 城宜嗣「細胞内での一酸化窒素の動態 NO Dynamics in Cellular System」第 55 回日本生物物理学会年会シンポジウム：実験と理論計算で明らかになってきた細胞環境での蛋白質間相互作用、2017 年 9 月 19 日、熊本 [2]
6. 當舎武彦「X 線自由電子レーザーを用いた時間分解結晶構造解析：酵素反応への応用」第 55 回日本生物物理学会年会 : 金属酵素の反応機構を理解するための多様な生物無機化学的アプローチ、2017 年 9 月 19 日、熊本 [2]
7. 杉本宏「病原菌のヘム輸送タンパク質の立体構造と機能」第 41 回日本鉄バイオサイエンス学会学術集会、2017 年 9 月 23 日、東京 [1]
8. Shiro, Y.: “Characterization of Coordination and Electronic Structures of Intermediates Appeared in NO Reduction by NO Reductases” *5th Ringberg Workshop on Structural Biology with FELs*, Munchen, Germany, Feb. 4 - 7 (2018) [2]
9. Tosha, T., Kubo, M.: “Time-resolved XFEL crystallography and *in crystallo* spectroscopy for probing reaction dynamics of respiratory metalloenzymes.” *5th Annual BioXFEL International Conference*, February 13, 2018, New Orleans, USA [2]
10. 當舎武彦「X 線自由電子レーザーを用いた時間分解結晶構造解析による酵素反応の追跡」日本化学会第 98 春季年会特別企画：学際的アプローチによる生命金属動態の解明と「生命金属科学」への展開、2018 年 3 月 23 日、船橋 [2]
11. H. Sugimoto, “Structural Basis of the ABC Heme Transporter in Iron Uptake System of Pathogenic Bacteria” 7th FEBS Special Meeting on ABC Proteins - ABC2018, Innsbruck, Austria, March 6-11 (2018) [4]
12. Shiro, Y.: “Coordination and Electronic Structures of Short-Lived Intermediate of Heme-Containing NO Reductases” 233rd ECS Meeting, Seattle, USA, May 13-17 (2018) [2, 4]
13. 澤井仁美：“ヒトの鉄吸収に関わる膜貫通型鉄還元酵素の立体構造に基づく生きた細胞での機能解析” 第 18 回日本蛋白質科学会年会 ワークショップ「金属イオンとタンパク質: その密接な関係が破綻するとき」、朱鷺メッセ（新潟）、2018 年 6 月 28 日 [4]
14. 城　宜嗣 : “時間分割測定法による一酸化窒素還元反応の分子機構解明” 第 18 回日本蛋白質科学会年会 ワークショップ「高分解能・動的構造解析によって明らかになりつつある生体エネルギー代謝系の仕組み」、朱鷺メッセ（新潟）、2018 年 6 月 28 日 [2, 4]
15. 當舎武彦：“光解離性基質を利用した時間分解 X 線結晶構造解析による酵素反応の追跡” 第 18

回日本蛋白質科学会年会ワークショップ「SACLA の先端技術がもたらす構造生物学研究のブレークスルー」、朱鷺メッセ（新潟）、2018 年 6 月 26 日 [2]

16. Shiro, Y.: “Coordination and Electronic Structures of Short-Lived Intermediate in Heme-Containing NO Reductases” *“Chemistry and Biology of Tetrapyrroles” Gordon Research Conference*, Newport, USA, July 15-20 (2018) [2, 1]
17. 澤井仁美：“SEC-SAXS 法を用いることで解明できた酸素センサータンパク質システム FixL/FixJ の全体像とシグナル伝達機構” 大阪大学蛋白質研究所セミナー／SPring-8 先端利用技術ワークショップ「第２回 SPring-8 における蛋白質構造生物学研究の現状と将来」、大阪大学、2018 年 8 月 10 日 [1]
18. 當舎武彦：”SACLA を利用した時間分解構造解析による酵素反応の観測” 新学術領域「中分子戦略」「分子夾雑化学」ジョイントシンポジウム第 21 回生命化学研究会　大阪大学　2018 年 9 月 8 日 [2]
19. H. Sugimoto “Structure Analysis of Radiation-Sensitive NO-bound State of Cytochrome P450nor Using XFEL at SACLA” 10th International Workshop on X-ray Radiation Damage to Biological Samples, Upton, USA, September 13-14 (2018) [2]
20. 當舎武彦：“生体システムがもつ効率的な一酸化窒素分解機構” （招待講演） 秋田大学理工学部生命科学コース特別講演会　秋田大学手形キャンパス　2018 年 9 月 14 日 [1, 4]
21. 當舎武彦：”Mechanism of Biological Nitric Oxide Reduction” 平成 30 年度化学系学協会東北大会 秋田大学手形キャンパス　2018 年 9 月 15 日 [2, 4]
22. 當舎武彦：”脱窒にみられる金属タンパク質複合体による効率的な連続化学反応” 第 56 回日本生物物理学会年会　岡山大学　2018 年 9 月 16 日 [2, 4]
23. 城　宜嗣：”Bacterial Nitric Oxide Reductases: Reaction Mechanism and Molecular Evolution” 第 56 回日本生物物理学会年会　Symposium “Developments and Future of Picobiology” 岡山大学 2018 年 9 月 16 日 [2, 4]
24. 城　宜嗣：“「生命金属科学」分野の創成” 錯体化学若手の会夏の学校 2018　アヤハレークサイドホテル（滋賀）、2018 年 9 月 22 日 [1, 2, 4]
25. 澤井仁美：“ヒトの鉄吸収機構を「膜タンパク質」と「生きた細胞」の研究により相互に理解する” 第 91 回日本生化学会年会 ワークショップ「生体金属の Magical Power とその研究最前線」、京都国際会館（京都）、2018 年 9 月 26 日 [4, 1]
26. T. Tosha “Regulation of nitric oxide dynamics in microbial denitrification” The International Symposium on Bioinorganic Chemistry 2018, Okazaki, Japan December 1, 2018 [1, 4]
27. Takeda, H., Nomura T., Tosha, T., Sugimoto, H., Kubo, M., Shiro, Y.: “Characterization of Sort-Lived Reaction Intermediates of Nitric Oxide Reductases by Time-Resolved Techniques” 9th Asian Biological Inorganic Chemistry (AsBIC-9), Natl. Univ. Singapore, December 12, 2018 [2, 4]
28. T. Tosha, E. Terasaka, K. Yamada, P.-H. Wang, H. Arai, H. Sugimoto, Y. Sugita and Y. Shiro “Nitric Oxide Dynamics Controlled by Formation of Protein Complex in Denitrification” 9th Asian Biological Inorganic Chemistry Conference (AsBIC9), Singapore, December 12, 2018 [1, 4]
29. 澤井仁美：“「鉄」のバイオサイエンス” 第 29 回 ST クラブ、じばさんびる（兵庫）、2019 年 1 月 28 日 [4, 1]
30. Y. Shiro: “Dynamics of Nitric Oxide in Bacterial Cellular Systems: NO Generation and Decomposition” *Japan-BIOCEV Symposium: Macromolecules; Structure, Function and Beyond*, Prague, Czech, Apr. 23 (2019) [1, 2]
31. T. Tosha “Elucidation of NO Reduction Mechanism in Soluble NO Reductase by Time-Resolved Crystallography with Photosensitive Caged Compound” *32nd European Crystallographic Meeting (ECM32)*, Vienna, Austria, Aug. 18-23 (2019) [1, 2]
32. Y. Shiro: “Dynamics of Nitric Oxide in Cellular Systems: NO Generation and Decomposition” *Korea-Taiwan-Japan Bioinorganic Chemistry Symposium 2019 (KTJ-BICS 2019)*, Taichung, Taiwan Nov. 12 -14 (2019) [1, 2]
33. 澤井仁美「病原菌の鉄獲得システムで機能するヘムセンサー蛋白質の多機能性とその構造的機序」　第 19 回日本蛋白質科学会年会／第 71 回日本細胞生物学会大会合同年次大会　ワークショップ「生命金属とタンパク質による細胞機能の協奏的制御」　2019 年 6 月 24 日、神戸 [1]
34. 澤井仁美「原子から細胞レベルの研究による鉄イオンの吸収メカニズムの理解と有効な鉄栄養強化食品成分の探索」　第 92 回日本生化学会大会　シンポジウム「生体内における Singularity

Elements としての生体金属の利用と制御」　2019 年 9 月 18 日、横浜 [1]

35. 城　宜嗣「分子構造を基盤にしたヘムタンパク質の機能解明～生命金属科学への展開をめざして～」　錯体化学会第 69 回討論会　貢献賞受賞講演　2019 年 9 月 22 日、名古屋
36. 城　宜嗣 “Molecular Mechanism of NO Reduction by Nitric Oxide Reductase in Cellular System” 第 57 回日本生物物理学会年会　シンポジウム「ヘム蛋白質の機能を司る構造・ダイナミクスとエネルギー流：実験と理論」　2019 年 9 月 26 日、宮崎 [1, 2]
37. 當舎武彦「実験と理論計算で解き明かす生体システムによる効率的な一酸化窒素分解機構」物性研短期研究会「理論タンパク質物性科学の最前線：理論と実験との密な協働」2020 年 2 月 28−29 日、東京大学柏キャンパス [1, 2]

(5) Patent applications（Research Category in [ ]）

N/A

(6) Collaborations including both inside and outside project（Research Category in [ ]）

1. 城　宜嗣（兵庫県立大）、杉田有治（理研）、八木　清（理研）: NO の生体内動態の分子動力学シミュレーションならびに電子状態解析 [2]
2. 城　宜嗣（兵庫県立大）、杉田有治（理研）、田村康一（理研）：ヘム膜輸送の分子動力学シミュレーション：ヘムインポーターとヘムエクスポーター [4]

(7) Hosted seminars and symposiums

1. 第１７回日本蛋白質科学会年会ワークショップ「生体内の金属動態：Structural Dynamics of Metals in Biology」（オーガナイザー：津本浩平、城宜嗣）、2017 年 6 月 22 日、仙台
2. 分子研研究会「生体金属動態」（オーガナイザー：青野重利、城宜嗣）2017 年 8 月 26～27 日、分子科学研究所、岡崎
3. 2017 年度生命科学系学会合同年次大会（ConBio2017），ワークショップ「X 線自由電子レーザーが捉えるタンパク質ダイナミクス研究の最前線」（オーガナイザー：南後恵理子、久保稔）、2017 年 12 月 6 日、神戸
4. 2017 年度生命科学系学会合同年次大会（ConBio2017），ワークショップ「生体金属動態の分子科学：「生命金属科学」への展開」（オーガナイザー：石森浩一郎、城宜嗣）、2017 年 12 月 6 日、神戸
5. 日本化学会第 98 春季年会　特別企画「学際的アプローチによる生命金属動態の解明と「生命金属科学」への展開」（オーガナイザー：青野重利、城宜嗣）2018 年 3 月 23 日、船橋
6. Symposium in International Conference on Porphyrins and Phthalocyanines (ICPP)-10, “Heme Enzymes: Functional Mechanisms in memory of Takashi Ogura” chaired by S. Nagano and T. Tosha, Munich, Germany 2018 年 7 月 3 日
7. 第 56 回日本生物物理学会年会　シンポジウム　“微生物における生命金属動態とその利用” オーガナイザー：古川良明、當舎武彦　岡山大学　2018 年 9 月 17 日（月）
8. 第 91 回日本生化学会年会 ワークショップ「生体金属の Magical Power とその研究最前線」　オーガナイザー：石森浩一郎、城　宜嗣　京都国際会館、2018 年 9 月 26 日
9. Microsymposium in 15th Asian Crystallographic Association Conference (AsCA 2018), “XFELs and Serial Crystallography” chaired by C. Darmanin and H. Sugimoto, Auckland, New Zealand, 2018 年 12 月 2-5 日
10. 城　宜嗣（年会長）、第 19 回日本蛋白質科学会年会／第 71 回日本細胞生物学会大会合同年次大会　2019 年 6 月 24 日、神戸
11. 澤井仁美、「生命金属科学」サテライトワークショップ「生体内における Singularity Elements としての生体金属の利用と制御」慶應義塾大学、2019 年 9 月 7 日
12. 澤井仁美、第９２回日本生化学会　シンポジウム 「生体内における Singularity Elements としての生体金属の利用と制御」パシフィコ横浜、2019 年 9 月 18 日

(8) Awards and honors

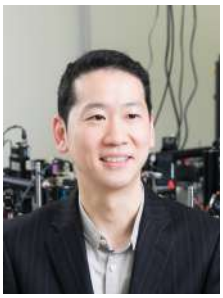
1. Rahman MD Mahfuzur: 2018 Student Research Achievement Award, 62nd Biophysical Society Meeting in San Francisco, 2018 月 2 月 20 日

2. Chai Gopalasingam：50 years of Synchrotron Radiation in the UK and its global impact (UKSR50), PDBe poster prize, 2018 年 6 月 29 日
3. Menega Ganasen：第 18 回日本蛋白質科学会年会　ポスター賞　2018 年 6 月 27 日
4. 澤井仁美：第 42 回日本鉄バイオサイエンス学会　学術奨励賞　2018 年 9 月 2 日
5. 武田英恵：第 56 回日本生物物理学会年会　学生発表賞　2018 年 9 月 16 日
6. Menega Ganasen：第 91 回日本生化学会大会　若手優秀発表賞　2018 年 9 月 24 日
7. 武田英恵：兵庫県立大　知の交流シンポジウム 2018　優秀ポスター賞　2018 年 9 月 26 日
8. 武田英恵：RIKEN Summer School 2018, Poster Award Chemistry Prize 2018 年 9 月 28 日
9. 武田英恵: 15th International Symposium on Applied Bioinorganic Chemistry (奈良)　Student Award、「NO-binding and Protonation Process in the Catalytic Reaction of Heme/non-heme Iron Nitric Oxide Reductase Proved by Time-Resolved Spectroscopic System」2019 年 6 月 5 日
10. 城　宜嗣：錯体化学会貢献賞、「分子構造を基盤にしたヘムタンパク質の機能解明～生命金属科学への展開をめざして～」2019 年 9 月 22 日

(9) Press releases

1. 合成酵素と分解酵素の協演―酵素タンパク質複合体形成による効率的な連続化学反応―、プレスリリース、2017 年 8 月 29 日
   https://www.riken.jp/press/2017/20170829_1/
2. 合成酵素と分解酵素が複合体を形成　生体内　効率的に NO 分解、科学新聞、2017 年 9 月 22 日
3. SACLA で酵素反応の可視化を実現 －生体内で起こる化学反応を原子レベルで見る－、プレスリリース、2017 年 11 月 17 日
   https://www.riken.jp/press/2017/20171117_2/
4. 生体内の酵素の動き解析 －佐用の理研、新薬開発に期待－、神戸新聞、2017 年 11 月 18 日
5. 安定な C-H 結合を室温で水酸化できる人工酵素の活性メカニズムを解明、日本経済新聞オンライン、2017 年 12 月 15 日
6. “土壌中の酸素濃度を感知して植物に窒素栄養を供給するタンパク質の全体構造を解明”
   http://www.sci.u-hyogo.ac.jp/news/1804112hitomisawai.pdf
   http://www.spring8.or.jp/ja/news_publications/press_release/2018/180411/
   https://news.liverpool.ac.uk/2018/04/11/synchrotron-science-could-give-soybeans-a-boost/
7. “貧血予防に新たな指針: ビタミンＣが鉄分の吸収を促進するメカニズムを原子レベルで解明”
   http://www.u-hyogo.ac.jp/outline/media/press/2018/monthly/pdf/20180820.pdf
   http://www.spring8.or.jp/ja/news_publications/press_release/2018/180820/

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Yuchiro KATO Chief Scientist RIKEN Cluster for Pioneering Research Nanoscale Quantum Photonics Laboratory 2-1 Hirosawa Wako Saitama 351-0198 JAPAN +81-(0)48-467-8152 yuichiro.kato@riken.jp 
Education	2000-2005 Department of Physics, University of California at Santa Barbara, USA 1996-2000 Department of Applied Physics, Keio University, Japan
Degrees	Ph.D. (2005) University of California at Santa Barbara M.A. (2003) University of California at Santa Barbara B.S. (2000) Keio University
Employment/research experience	2017- Chief Scientist, Nanoscale Quantum Photonics Laboratory, RIKEN Cluster for Pioneering Research 2016- Team Leader, Quantum Optoelectronics Research Team, RIKEN Center for Advanced Photonics 2016-2017 Associate Chief Scientist, Nanoscale Quantum Photonics Laboratory, RIKEN 2007-2016 Associate Professor, Institute of Engineering Innovation, The University of Tokyo 2005-2007 Postdoctoral Scholar, Chemistry Department, Stanford University Additional positions 2016- Visiting Associate Professor, The University of Tokyo
Awards and honors	Young Scientists' Prize in the Commendation for Science and Technology (Minister of Education, Culture, Sports, Science and Technology, Japan) (2009) Newcomb-Cleveland Prize (American Association for the Advancement of Science) (2005)
Academic activities	Member, American Physical Society Member, American Chemical Society Member, Optical Society of America Member, Japan Society for Applied Physics Member, The Fullerenes, Nanotubes and Graphene Research Society Member; Physical Society of Japan Member; The Japan Society of Vacuum and Surface Science Symposium executive committee, The Fullerenes, Nanotubes and Graphene Research Society (2013-) Program committee, International Conference on Nano-photonics and Nano-optoelectronics (ICNN) (2019-2020)

	Organizer, Fundamental Optical Processes in Semiconductors (FOPS) (2019) Organizing committee chair, 7th Workshop on Nanotube Optics and Nanospectroscopy (WONTON) (2018) International advisory & program committee member, 8th International Conference on the Physics & Applications of Spin Phenomena in Solids (PASPS VIII) (2014) International advisory committee member, 7th International School and Conference on Spintronics and Quantum Information Technology (Spintech 7) (2013) Program committee member, 6th International School and Conference on Spintronics and Quantum Information Technology (Spintech 6) (2011)

(1) Participants

Yuichiro Kato（加藤 雄一郎）	主任研究員
Wataru Terashima（寺嶋 亘）	研究員
Daiki Yamashita（山下 大喜）	特別研究員
Nan Fang（方 楠）	特別研究員
Zhen Li（李 臻）	特別研究員
Akihiro Ishii（石井 晃博）	特別研究員
Shunsuke Tanaka（田中 駿介）	特別研究員
Keigo Otsuka （大塚 慶吾）	訪問研究員
Widianta Gomulya	訪問研究員
Alka Sharma	訪問研究員
Hidenori Machiya（町屋 秀憲）	研修生

(2) Original papers（Research Category in [ ]）

1. A. Ishii, X. He, N. F. Hartmann, H. Machiya, H. Htoon, S. K. Doorn, Y. K. Kato, "Enhanced single photon emission from carbon nanotube dopant states coupled to silicon microcavities", Nano Lett. **18**, 3873 (2018). [5]
2. W. Gomulya, H. Machiya, K. Kashiwa, T. Inoue, S. Chiashi, S. Maruyama, Y. K. Kato, "Enhanced Raman scattering of graphene using double resonance in silicon photonic crystal nanocavities", Appl. Phys. Lett. **113**, 081101 (2018). [5]
3. T. Uda, S. Tanaka, Y. K. Kato, "Molecular screening effects on exciton-carrier interactions in suspended carbon nanotubes", Appl. Phys. Lett. **113**, 121105 (2018). [5]
4. S. Tanaka, K. Otsuka, K. Kimura, A. Ishii, H. Imada, Y. Kim, Y. K. Kato, "Organic molecular tuning of many-body interaction energies in air-suspended carbon nanotubes", J. Phys. Chem. C **123**, 5776 (2019). [5]
5. K. Otsuka, A. Ishii, Y. K. Kato, "Super-resolution fluorescence imaging of carbon nanotubes using a nonlinear excitonic process", Opt. Express **27**, 17463 (2019). [5]
6. A. Ishii, H. Machiya, Y. K. Kato, "High efficiency dark-to-bright exciton conversion in carbon nanotubes", Phys. Rev. X **9**, 041048 (2019). [5]

(3) Reviews and books（ Research Category in [ ] ）

1. A. Ishii, H. Machiya, T. Uda, Y. K. Kato, "Exciton Physics in Single-Wall Carbon Nanotube Photonic and Optoelectronic Devices", in *Handbook of Carbon Nanomaterials* edited by R. B. Weisman and J. Kono (World Scientific Publishing, Singapore, 2019) Vol. 9, Optical Properties of Carbon Nanotubes, Part I: A Volume Dedicated to the Memory of Professor Mildred S Dresselhaus, Chap. 7, p. 269-396. [5]

(4) Invited presentations（ Research Category in [ ] ）

1. A. Ishii, T Uda, Y. K. Kato: "Room-temperature single photon emission from micrometer-long air-suspended carbon nanotubes", 233rd Electrochemical Society Meeting, Seattle, Washington, USA , May (2018). [5]
2. Y. K. Kato: "Single-carbon-nanotube photonics and optoelectronics", OSA Advanced Photonics Congress, Zurich, Switzerland, July (2018). [5]
3. Y. K. Kato: "Air-suspended carbon nanotubes for nanoscale quantum photonics", International Workshop on Nanocarbon Photonics and Optoelectronics (NPO2018), Savonlinna, Finland, August (2018). [5]

4. Y. K. Kato: “Single-carbon-nanotube photonics and optoelectronics”, Conference on Lasers and Electro-Optics (CLEO2019), San Jose, CA, USA, May (2019). [5]
5. S. Tanaka, K. Otsuka, K. Kimura, A. Ishii, H. Imada, Y. Kim, Y. K. Kato: “Organic molecular tuning of many-body interaction energies in air-suspended carbon nanotubes”, 235th Electrochemical Society Meeting, Dallas, Texas, USA, May (2019). [5]
6. Y. K. Kato: “Exciton Physics in Air-Suspended Carbon Nanotubes”, International Conference on the Science and Application of Nanotubes and Low-Dimensional Materials (NT19), Wurzburg, Germany July (2019). [5]
7. A. Ishii, H. Machiya, Y. K. Kato: “High efficiency dark-to-bright exciton conversion in carbon nanotubes”, Fundamental Optical Processes in Semiconductors (FOPS), Banff, Canada, August (2019). [5]
8. Y. K. Kato, “Exciton physics in individual carbon nanotubes”, 日本物理学会2019年秋季大会（物性）、岐阜県岐阜市、2019年9月.[5]
9. 加藤雄一郎： “今でしょ！その場で作る機能性材料”、第9回CSJ化学フェスタ、東京都江戸川区、2019年10月. [5]
10. Y. K. Kato: “Single-carbon-nanotube photonics and optoelectronics”, Optics & Photonics Taiwan, International Conference (OPTIC2019), Taichung City, Taiwan, December (2019). [5]

(5) Patent applications（ Research Category in [ ] ）

N/A

(6) Collaborations including both inside and outside project（ Research Category in [ ] ）
1. Y. K. Kato、S. K. Doorn (Los Alamos National Laboratory) : Carbon nanotube dopant states coupled to silicon microcavities [5]
2. 加藤 雄一郎、丸山 茂夫（東京大学）：グラフェンとフォトニック結晶の光結合 [5]
3. 加藤 雄一郎、金 有洙（理研）：有機分子とカーボンナノチューブの界面 [5]

(7) Hosted seminars and symposiums
1. 7th Workshop on Nanotube Optics and Nanospectroscopy (WONTON18), Hakone, Japan, July 8-12 (2018).
2. JSPS-DFG Bilateral Meeting on Carbon Nanotube Optics and Nanospectroscopy, Hakone, Japan, July 8-13 (2018).
3. 理研-東京大学カーボンナノチューブミニワークショップ、和光市、2018年11月7日.
4. Seminar, “Sub-wavelength modifications in silicon-on-insulator microring resonators for enhanced sensing”, Armandas Balcytis, (Ph.D. Student, Center for Micro-Photonics, Swinburne University of Technology, Wako, Japan, November 14 (2018).
5. セミナー、「Determination of the position of a single nuclear spin from free nuclear precessions detected by a solid-state quantum sensor」、佐々木　健人（慶應義塾大学理工学部物理情報工学科伊藤研究室　博士課程）、和光市、2019年1月29日.
6. セミナー、「Fundamentals and applications of microresonator frequency combs」、藤井　瞬（慶應義塾大学理工学部電子工学科田邉研究室　博士課程）、和光市、2019年1月31日.
7. セミナー、「高Q値フォトニック結晶ナノ共振器を用いた量子ドット共振器量子電磁力学」、車一宏（東京大学工学系研究科電気系工学専攻岩本研究室　博士課程）、和光市、2019年2月19日.
8. セミナー、「自己形成IgAs/GaAs量子ドットを用いた単一プラズモン源に関する研究」、玉田　晃（東京大学工学系研究科電気系工学専攻岩本研究室　博士課程）、和光市、2019年2月19日.
9. セミナー、“ナノマイクロ構造を用いた熱ふく射のスペクトル制御とTPV発電への応用に関する研究”、磯部 和真 (東京工業大学理工学研究科機械制御システム専攻花村研究室 博士課程)、和光市、2019年2月28日.
10. セミナー、“Lasing characteristics of nanocavity Raman silicon lasers”、山下 大喜 (大阪府立大学工学研究科電子物理工学分野高橋研究室博士課程)、和光市、2019年3月13日.

11. Seminar, “Tuning the emission properties of (6,5) Carbon Nanotubes with Strong Coupling in Cavities, Doping and sp3 Functionalization”, Jana Zaumseil 博士 (Professor, Faculty of Chemistry & Earth Science, Heidelberg University, Germany), Wako, October 5 (2019).
12. Seminar, “Low dimensional structures and devices: Semiconductor quantum dots and nanocrystals”, Fong Chee Fai 博士 (Research Fellow, Nanyang Technological University, Singapore) , November 11 (2019).
13. Seminar, “Air-suspended, sp3-functionalized carbon nanotubes”, Nicolas Frederic Zorn, (PhD Student, Faculty of Chemistry & Earth Science, Heidelberg University, Germany), Wako, March 31 (2020).

(8) Awards and honors

1. 石井晃博：“第 10 回研究奨励賞（桜舞賞）”、国立研究開発法人理化学研究所、2019 年 3 月 12 日.

(9) Press releases

1. RIKEN research highlight, “Carbon nanotubes on holey silicon make bright source of single photons”, 2018 年 7 月 27 日.
   https://www.riken.jp/en/news_pubs/research_news/20180727_FY20180020/
2. RIKEN RESARCH, “Enhanced emission of single photons realized”, p18, WINTER (2018).
3. 理研プレスリリース、「暗い励起子から明るい励起子への変換機構を解明　ーカーボンナノチューブの発光効率向上への新指針ー」、2019 年 12 月 6 日.
   https://www.riken.jp/press/2019/20191206_1/index.html
4. 化学工業日報、「CNT の発光効率向上に指針」、2019 年 12 月 9 日.
5. オプトロニクスオンライン「理研，CNT の発光効率向上へ新知見」、2019 年 12 月 9 日.
6. Laser Focus World Japan、「理研、暗い励起子から明るい励起子への変換機構を解明」、2019 年 12 月 9 日.
   http://www.optronics-media.com/news/20191209/61716/
7. ナノテクジャパン、「暗い励起子から明るい励起子への変換機構を解明　～カーボンナノチューブの発光効率向上への新指針～」、2019 年 12 月 20 日.
   https://www.nanonet.go.jp/ntj/topics_ntj/?mode=article&article_no=4968
8. RIKEN research highlight, “Dark excitons can make a high contribution to light emission from nanotubes”, 2020 年 3 月 6 日.
   https://www.riken.jp/en/news_pubs/research_news/rr/20200306_2/

Fujii Laboratory, Tokyo Institute of Technology
藤井研究室, 東京工業大学

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Masaaki FUJII Professor Tokyo Institute of Technology Insititute of Innovative Research R1-15 4259 Nagatsuta-cho,Midori-ku, Yokohama 226-8503 JAPAN +81-(0)45-924-5250 mfujii@res.titech.ac.jp 
Education	1982-1985 Graduate School of Science, Tohoku University 1979-1982 Tohoku University, Faculty of Science, Department of Chemistry
Degrees	Dr. Sci. (1987) Tohoku University M. Sci. (1984) Tohoku University B. Sci. (1982) Tohoku University
Employment/research experience	2003- Professor of Tokyo Institute of Technology 1999-2003 Director of Laser Research Center for Molecular Science 1997-2003 Professor of Institute for Molecular Science 1993-1997 Associate Professor, Waseda University, Japan 1985-1993 Research Associate, Department of Chemistry, Faculty of Science, Tohoku University, Japan <u>Additional post</u> 1988 Visiting Scientist by US-Japan Collaboration on Solar Energy Transfer (Cornell University, Professor A. C. Albrecht) 2019- Visiting Senior Researcher of RIKEN
Awards and honors	Chemical Society of Japan, Award for the Young Chemist (1992) Award by Yamashita Memorial Foundation for Science and Engineering (1992) Morino Foundation for Molecular Science (1996) Teshima Foundation Prize for the Best Research Paper for Science and Technology (2007) The New Technology Development Foundation, Ichimura Prize (2008) Chemical Society of Japan, Award for Creative Work (2014) The Spectroscopical Society of Japan Award (2015) Distinguished Scientist Awards of the Japan Society for Molecular Science (2018) Humboldt Research Awards (2019)
Academic activities	Member; Chemical Society of Japan Member; American Chemical Society Member; Spectroscopical Society of Japan Member; Japan Society for Molecular Science Trustée of The Spectroscopical Society of Japan (2014-2018) President, Japan Society for Molecular Science (2014-2016) Project Leader of Priority Area (477) （2007−2012）

	Project Leader and Coordinator in Core-to-Core Program (2010-2015) Vice Chairperson, Gordon Research Conference on Molecular an Ionic Clusters (2008) Chairperson, Molecular an Ionic Clusters Conference (2010)

(1) Participants

Masaaki Fujii （藤井 正明）	教授（東工大・化学生命科学研究所）
Shun-ichi Ishiuchi（石内 俊一）	准教授（東工大・化学生命科学研究所）
Mitsuhiko Miyazaki（宮﨑 充彦）	助教（東工大・化学生命科学研究所）
Keisuke Hirata（平田 圭佑）	助教（東工大・化学生命科学研究所）
James M. Lisy	特任教授（東工大・科学技術創成研究院）
Otto Dopfer	特任教授（東工大・科学技術創成研究院）
Anne Zehnacker-Rentien	特任教授（東工大・科学技術創成研究院）
Christophe Jouvet	特任教授（東工大・科学技術創成研究院）
Sotiris S. Xantheas	特任教授（東工大・科学技術創成研究院）
Mattanjah S. de Vires	特任教授（東工大・科学技術創成研究院）
Yuki Konno（今野 裕貴）	修士課程学生（東工大・化学生命科学研究所）
Kazuya Tsuruta（雀田 知弥）	修士課程学生（東工大・化学生命科学研究所）
Keisuke Yamaguchi（山口 佳祐）	修士課程学生（東工大・化学生命科学研究所）
Remina Otsuka（大塚 玲美奈）	修士課程学生（東工大・化学生命科学研究所）
Kenichi Kasai（笠井 賢一）	修士課程学生（東工大・化学生命科学研究所）
Tairiku Kamiya（紙谷 大陸）	修士課程学生（東工大・化学生命科学研究所）
Mizuki Tabata（田端 みずき）	修士課程学生（東工大・化学生命科学研究所）
Masato Tamura（田村 将人）	修士課程学生（東工大・化学生命科学研究所）
Eiko Sato（佐藤 映虹）	修士課程学生（東工大・化学生命科学研究所）
Takumi Negoro（根来 拓己）	修士課程学生（東工大・化学生命科学研究所）
Sohichiroh Mitsui（三井 聡一郎）	修士課程学生（東工大・化学生命科学研究所）
Yuta Mori（森 優太）	修士課程学生（東工大・化学生命科学研究所）
Naoya Takeda（武田 直也）	学部学生 （東工大・生命理工学院）
Yoshimitu Fukui（福井 義光）	学部学生 （東工大・生命理工学院）
Tatsuya Yoshinaga（吉永 達哉）	学部学生 （東工大・生命理工学院）

(2) Original papers（Research Category in [ ]）

1. T. Sekiguchi, M. Tamura, H. Oba, P. Çarçarbal, R. R. Lozada-Garcia, A. Zehnacker-Rentien, G. Grégoire, S. Ishiuchi, M. Fujii, “Molecular Recognition by a Short Partial Peptide of the Adrenergic Receptor: A Bottom-Up Approach”, *Angew. Chem. Int. Ed.* **57**, 5626 (2018). (**Journal Cover**) [1,4]
2. A. Bouchet, J. Klyne, S. Ishiushi, O. Dopfer, M. Fujii, A. Zehnacker-Rentien, “Stereochemistry-dependent structure of hydrogen-bonded protonated dimers: the case of 1-amino-2-indanol”, *Phys. Chem. Chem. Phys.* **20**, 12430 (2018) . [1,4]
3. W. Y. Sohn, J. J. Kim, M. Jeon, T. Aoki, S. Ishiuchi, M. Fujii, H. Kang, “Entropic effects make a more tightly folded conformer of a β-amino acid less stable: UV-UV hole burning and IR dip spectroscopy of L-β^3-homotryptophan using a laser desorption supersonic jet technique”, *Phys. Chem. Chem. Phys.* **20**, 19979 (2018) . [1,2,4]
4. M. Miyazaki, N. Washio, M. Fujii, “Electron-proton transfer mechanism of excited-state hydrogen transfer in phenol–$(NH_3)_n$ ($n = 5$) studied by delayed ionization detected femtosecond time-resolved NIR spectroscopy”, *Chem. Phys.* **515**, 580 (2018). [1,2,4]
5. J. Klyne, A. Bouchet, S. Ishiuchi, M. Fujii, M. Schneider, C. Baldauf, O. Dopfer, “Probing chirality recognition of protonated glutamic acid dimers by gas-phase vibrational spectroscopy and first-principles simulations”, *Phys. Chem. Chem. Phys.* **20**, (2018) 28452. [1,4]
6. S. Ishiuchi, Y. Sasaki, J. M. Lisy, M. Fujii, “Ion-peptide interactions between alkali metal ions and a termini-protected dipeptide; Modeling a portion of the selectivity filter in K^+ channels”, *Phys. Chem. Chem. Phys.* **21**, 561 (2019). (**Journal Cover**) [1,4]
7. M. Tamura, T. Sekiguchi, S. Ishiuchi, A. Zehnacker-Rentien, M. Fujii, “Can the Partial Peptide SIVSF of the β_2-Adrenergic Receptor Recognize Chirality of the Epinephrine Neurotransmitter?” *J. Phys. Chem. Lett.* **10**, 2470 (2019). (**Journal Cover**) [1,4]
8. S. Ishiuchi, H. Wako, S. S. Xantheas, M. Fujii, “Probing the selectivity of Li^+ and Na^+ cations on noradrenaline at the molecular level”, *Faraday Discuss.* **217**, 396 (2019). [1,4]

9. M. Miyazaki, K. Chatterjee, K. Hattori, R. Otsuka, S. Ishiuchi, O. Dopfer, M. Fujii, "Ionization-Induced π → H Site Switching in Resorcinol-Ar_n (n = 1 and 2) Clusters Probed by Infrared Spectroscopy" *J. Phys. Chem. A* **132**, 6828 (2019). [1,2,4]
10. S. Ishiuchi, J. Kamizori, N. Tsuji, M. Sakai, M. Miyazaki, C. Dedonder, C. Jouvet, and Masaaki Fujii, "Excited state hydrogen transfer dynamics in phenol–(NH3)2 studied by picosecond UV-near IR-UV time-resolved spectroscopy", *Phys. Chem. Chem. Phys*., **22**, 5740 (2020). [1,2,4]
11. R. Otsuka, K. Hirata, Y. Sasaki, J. M. Lisy, S. Ishiuchi, M. Fujii, "Alkali and alkaline earth metal ions complexes with a partial peptide of the selectivity filter in K^+ channels studied by a cold ion trap infrared spectroscopy" *ChemPhysChem* in press, DOI: 10.1002/cphc.202000033 (**Journal Cover**). [1,4]

(3) Reviews and books（ Research Category in [ ] ）

1. M. Fujii, O. Dopfer, "Time-Resolved Study on Photo-Initiated Isomerization of Clusters", Chapter 13 in "Physical Chemistry of Cold Gas-Phase Functional Molecules and Clusters" 2019, Springer, p.367-395. [1,2,4]
2. T. Ebata and M. Fujii (Editor), "Physical Chemistry of Cold Gas-Phase Functional Molecules and Clusters", 2019, Springer. [1,2,4]

(4) Invited presentations（ Research Category in [ ] ）

1. M. Fujii, "Chiral recognition in protonated molecular clusters studied by mass-coupled IR-UV double resonance spectroscopy with cold ion trap", 22nd International Mass Spectrometry Conference 2018 (IMSC2018), Fortezza da Basso, Florence, 2018 Aug, Italy (2018). [1, 4]
2. M. Fujii, "Bottom-Up Approach to Biological Molecular Recognition – Electrospray-Cold Ion Trap Laser Spectroscopy on Binding Motif of Adrenergic Receptor", State Key Laboratory Seminar of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, CAS, 2018 Nov., China (2018). [1,4]
3. 田村将人 :「エレクトロスプレー・冷却イオントラップ法によるアドレナリン受容体部分ペプチド（SIVSF）・リガンド錯体の気相分光―分子認識に対する光学異性効果」, 日本分光学会第 14 回先端レーザー分光シンポジウム, 2019 年 1 月 16 日, 理研 (2019). [1,4]
4. 石内俊一 :「計測系から見た分子集合体の機能計測―イオントラップ分光」, 日本化学会第 99 春季年会, 甲南大学 (2019). [1,4]
5. M. Miyazaki, "Water migration dynamics in hydrated clusters - Real-time observation by time-resolved IR spectroscopy", 日本化学会第 99 春季年会, 甲南大学 (2019). [1,2,4]
6. M. Fujii, "Bottom-Up Approach to the Molecular Recognition of Adrenaline Receptor by Electrospray-Cold Ion Trap IR Laser Spectroscopy" 10th International Conference on Advanced Vibrational Spectroscopy, The University of Auckland, Auckland, 2019 Jul., New Zealand (2019). [1,4]
7. M. Fujii, "Bottom-up Approach to Molecular Recognition in Biological Systems: ESI / Cold Ion Trap Spectroscopy" International Symposium Frontiers in Cluster Science: Structure and Dynamics, TU Berlin, Berlin, 2019 Nov., Germany. [1,4]
8. S. Ishiuchi, "Cold Ion Trap Spectroscopy for Molecular Recognition Systems", Molecular and Ionic Clusters Gordon Research Conference, Ventura Beach Marriott, Ventura, CA, 2020 Jan., the U. S (2020). [1,4]

(5) Patent applications（ Research Category in [ ] ）

N/A

(6) Collaborations including both inside and outside project（ Research Category in [1, 4] ）

1. 藤井正明、石内俊一、北尾彰朗（東工大生命理工）：オキシトシンの構造と赤外スペクトルの理論計算 [1]
2. 藤井正明、石内俊一、八木清、杉田有治（理研）：SIVSF ペプチドの構造と赤外スペクトルの理論計算ならびに計算手法開発 [1]

3. 藤井正明、石内俊一、Sotiris Xantheas (PNNL, US 及び東工大 WRHI) ：Li 塩の薬理作用

(7) Hosted seminars and symposiums

1. Tokyo Tech World Research Hub Initiatives International Workshop, “Advanced Laser Spectroscopy for Soft Molecular Systems”, 2018 30 Nov., Suzukakedai campus, Tokyo Institute of Technology, Japan (2018).
2. Tokyo Tech World Research Hub Initiatives International Workshop, “Advanced Laser Spectroscopy for Soft Molecular Systems”, 2019 15 Nov., Suzukakedai campus, Tokyo Institute of Technology, Japan (2019).

(8) Awards and honors

1. 藤井 正明：“第 9 回分子科学会賞”、分子科学会、2018 年 9 月 12 日.
2. 田村 将人：“大隅ジャーナル賞”、東京工業大学、2019 年 6 月 10 日.
3. 藤井 正明：“フンボルト賞”、アレクサンダー・フォン・フンボルト財団、2019 年 6 月 27 日
4. 石内 俊一：“第 4 回分子科学国際学術賞”、分子科学会、2019 年 9 月 17 日.
5. 大塚 玲美奈：“第 13 回分子科学会優秀講演賞”、分子科学会、2019 年 10 月 30 日.
6. 田村 将人：“第 13 回分子科学会優秀ポスター賞”、分子科学会、2019 年 10 月 30 日.
7. 田端 みずき：“第 13 回分子科学会優秀ポスター賞”、分子科学会、2019 年 10 月 30 日.

(9) Press releases

N/A

Institute for Molecular Science, Yamamoto Group
分子科学研究所，山本グループ

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Hiroshi, YAMAMOTO  Professor Research Center of Integrative Molecular Science, Institute for Molecular Science, National Institutes of Natural Sciences 38 Nishigounaka, Myodaiji, Okazaki, Aichi 444-8585 JAPAN +81-(0)564-55-7334 yhiroshi@ims.ac.jp
Education	1993-1998 Graduate School of Science, The University of Tokyo 1991-1993 The University of Tokyo, Faculty of Science, Department of Chemistry 1989-1991 The University of Tokyo, College of General Education
Degrees	Dr. Sci. (1998) The University of Tokyo M. Sci. (1995) The University of Tokyo B. Sci. (1993) The University of Tokyo
Employment/research experience	2012- Professor, Institute for Molecular Science, National Institutes of Natural Sciences 2000-2012 Research Scientist, Condensed Molecular Materials Laboratory, RIKEN 1999-2000 Special Postdoctoral Researcher, Condensed Molecular Materials Laboratory, RIKEN 1998-1999 Research Associate, Department of Physics, Faculty of Science, Gakushuin University <u>Additional post</u> 2013-2019 Visiting Senior Scientist, RIKEN 2015-2020 Visiting Professor, Tohoku University 2012-2019 Visiting Professor, Tokyo Institute of Technology 2016 Visiting Professor, Angers University 2011 Visiting Professor, Renne University 1
Awards and honors	The NAGAI Foundation for Science ＆ Technology Academic award(2020) Chemical Society of Japan Academic award (2019) Japan Society for the Promotion of Science, Grants-in-Aid for Scientific judging committee award (2016) RIKEN Incentive award (2010) Japan Society for Molecular Science encouraging prize(2009) CrystEngComm Prize （RSC Publishing） (2009)
Academic activities	Member; Chemical Society of Japan Member; Physical Society of Japan Member; Japan Society of Molecular Science Member; The Japan Society of Applied Physics

	Standing executive secretary; Tokai division, Chemical Society of Japan (2015-2017) Project general manager; Section B, 142th University-Industry Cooperative Research Committees, Japan Society for the Promotion of Science (2014-2018) Executive secretary; Physical chemistry division, Chemical Society of Japan (2014-2018) Secretary; The 12th International Symposium on Crystalline Organic Metals, Superconductors and Ferromagnets (2017) Steering committee member; Japan Society of Molecular Science (2018-) Vice chair; Division 7, Physical Society of Japan (2018-2019) Chair; Division 7, Physical Society of Japan (2019-2020) Chair; The 80th Okazaki conference “Chirality-Induced Spin Selectivity and its related phenomena” (2019) Session organizer; Materials Research Meeting 2019 (2019)

(1) Participants

Hiroshi Yamamoto（山本 浩史） 教授
Masayuki Suda （須田 理行） 助教
Genta Kawaguchi （川口 玄太） 特任助教

(2) Original papers（Research Category in [ ]）

1. G. Kawaguchi, A. A. Bardin, M. Suda, M. Uruichi, and H. M. Yamamoto: "An Ambipolar Superconducting Field-Effect Transistor Operating above Liquid Helium Temperature", Adv. Mater., **2018**, 1805715 (2018). [5, 1]
2. Y. Kawakami, T. Amano, Y. Yoneyama, Y. Akamine, H. Itoh, G. Kawaguchi, H. M. Yamamoto, H. Kishida, K. Itoh, T. Sasaki, S. Ishihara, Y. Tanaka, K. Yonemitsu, and S. Iwai: "Non-linear charge oscillation driven by single-cycle light-field in an organic superconductor", Nature Photonics, **12**, 474 (2018). [5, 1]
3. G. Kawaguchi and H. M. Yamamoto: "Control of Organic Superconducting Field-Effect Transistor by Cooling Rate", Crystals, **9**, 605 (2019). [5, 1]
4. Tianchai Chooppawa, Supawadee Namuangruk, Hiroshi M. Yamamoto, Vinich Promarak and Paitoon Rashatasakhon: "Synthesis, characterization, and hole-transporting properties of benzotriazatruxene derivatives", J. Mater. Chem. C, **7**, 15035 (2019). [5]
5. M. Suda, Y. Thathong, V. Promarak, H. Kojima, M. Nakamura, T. Shiraogawa, M. Ehara and H. M. Yamamoto: "Light-driven Molecular Switch for Reconfigurable Spin Filters", Nature Commun., **10**, 2455 (2019). [4]
6. Hiroshi Ito, Yusuke Edagawa, Jiang Pu, Hiroki Akutsu, Masayuki Suda, Hiroshi M. Yamamoto, Yoshitaka Kawasugi, Rie Haruki, Reiji Kumai, and Taishi Takenobu: "Electrolyte-Gating-Induced Metal-Like Conduction in Nonstoichiometric Organic Crystalline Semiconductors under Simultaneous Bandwidth Control", Phys. Status Solidi PRL, **2019**, 1900162 (2019). [5, 1]
7. Y. Kawasugi, K. Seki, S. Tajima, J. Pu, T. Takenobu, S. Yunoki, H. M. Yamamoto, and R. Kato: "Two-dimensional ground-state mapping of a Mott-Hubbard system in a flexible field-effect device", Sci. Adv. **5**, eaav7282 (2019) [5, 1]
8. Tianchai Chooppawa, Masayuki Suda, Mikio Uruichi, Manaschai Kunaseth, Supawadee Namuangruk, Paitoon Rashatasakhon, and Hiroshi M. Yamamoto: "Development of highly soluble perylenetetracarboxylic diimide derivative for n-type monolayer field-effect-transistor", Mol. Cryst. Liq. Cryst., 669, 94 (2019) [5].

(3) Reviews and books（ Research Category in [ ] ）

1. H. M. Yamamoto, M. Suda, Y. Kawasugi,: "Organic phase-transition transistor with strongly correlated electrons", Jpn. J. Appl. Phys., **57**, 03EA02 (2018). [5, 1]
2. 山本浩史、須田理行："光で制御する超伝導　～光応答性電気二重層トランジスタ～"、物理学会誌、**73**、143-147 (2018). [5, 1]
3. 須田理行、山本浩史："分子モーターを用いた再構成可能スピン偏極デバイス"、応用物理、**89**, 203-207. [4]

(4) Invited presentations（ Research Category in [ ] ）

1. H. M. Yamamoto: "Field-effect-transistors with phase-transitions", PACCON2018, Hat Yai, Thailand (Feb. 2018). [5,1]
2. H. M. Yamamoto: "Molecular conductors for electronics", ICCC2018, Sendai, Japan (Aug. 2018). [5,1]
3. M. Suda, "Superconducting FETs based on organic strongly correlated materials," Gordon Research Conference—Conductivity and Magnetism in Molecular Materials—, Rhode Island, U.S.A., (Aug. 2018). [5,1]

4. H. M. Yamamoto: “Electronic Phase Transition at an Organic Field-Effect-Transistor Interface”, 2018 Int’l Roundtable of NanoScience and NanoTechnology Symposium, Shanghai, China (Sep. 2018). [5,1]
5. H. M. Yamamoto: “Organic Field-Effect-Transistors based on Charge-Transfer Salts”, Organic Semiconductors, Conductors, and Electronics, Aichi, Japan (Oct. 2018). [5,1]
6. H. M. Yamamoto: “Electronic phase transitions at an organic field-effect-transistor interface”, NCTU workshop, Shinchu, Taiwan (Oct. 2018). [5,1]
7. H. M. Yamamoto: “Organic Field-Effect-Transistor with Strongly Correlated Electrons”, NanoThailand2018, Bangkok, Thailand (Dec. 2018). [5,1]
8. H. M. Yamamoto: “Electronic phase transitions at an organic field-effect-transistor interface” NanoTalk, NANOTEC, Bangkok, Thailand (Feb. 2019). [5,1]
9. 山本浩史：“量子位相に着目した有機デバイスの新展開”、日本化学会年会特別企画、兵庫県神戸市、2019 年 3 月. [5,1]
10. 山本浩史：“Studies on Phase-Transition Devices Based on Organic Mott Insulators”、日本化学会年会学術賞受賞特別講演、兵庫県神戸市、2019 年 3 月. [5,1]
11. 須田理行,「 界面光異性化分子を用いた電子物性の光制御」, 日本物理学会第 74 回年次大会シンポジウム「有機分子と表面の出会いがもたらす多体相関物性」, 福岡（日本）, 2019 年 3 月. [5,1]
12. 須田理行,「 分子キラリティ制御に基づくスピン偏極電流の生成と外場制御」, 早稲田大学高等研究所「Top Runner's Lecture Collection of Science—物質の構造と対称性がもたらす電磁交差応答の最前線：マルチフェロイクスとスピントロニクス—」, 早稲田大学, 東京（日本）, 2019 年 4 月[4]
13. Hiroshi Yamamoto, “Light-driven molecular switch for reconfigurable spin filters”, ANSCSE2019, Chiang Mai, Thailand (Jun. 2019)
14. 山本浩史：“有機強相関トランジスタを用いた物性科学”、第 4 回固体化学フォーラム研究会、愛知県岡崎市、2019 年 6 月. [5,1]
15. 山本浩史：“薄膜デバイスを用いた有機強相関電子系の物性制御”、名古屋大学理学研究科講演会、愛知県名古屋市、2019 年 7 月. [5,1]
16. Hiroshi Yamamoto, “Light-driven molecular switch for reconfigurable spin filters”, 17th Japan-Korea Symposium on Molecular Science, Nagoya (Jul. 2019). [4]
17. Hiroshi Yamamoto, “Band-filling and Band-width control for κ-(BEDT-TTF)2Cu[N(CN)2]X embedded in field effect devices”, ISCOM2019, Tomar, Portugal (Sep. 2019). [5,1]
18. Hiroshi Yamamoto, “Spin Filter Driven By Molecular Motor”, 5th Japan-Thai workshop on TCC2019, Yokohama (Oct. 2019). [4]
19. Hiroshi Yamamoto, “Light-driven Molecular Switch for Reconfigurable Spin Filters”, Chirality@The Nanoscale, Ascona, Switzerland (Oct. 2019). [4]
20. 須田理行,「 機能性有機単分子膜を利用した固体物性の外場制御」, 第 10 回分子アーキテクトニクス研究会, 福岡（日本）,2019 年 11 月. [5,1]

(5) Patent applications（ Research Category in [ ] ）

1. 戸川欣彦、宍戸寛明、山本浩史：“キラリティ検出装置、キラリティ検出方法、分離装置及び分離方法”、特願 2019-092958、2019 年 5 月 16 日. [4,5]
2. 戸川欣彦、宍戸寛明、山本浩史：“キラル物質装置”、特願 2019-092959、2019 年 5 月 16 日.[4,5]

(6) Collaborations including both inside and outside project（ Research Category in [ ] ）

1. 山本浩史、川椙義高、柚木清司、関和弘（理化学研究所）：ドープモット絶縁体の基底状態計算 [1]
2. 山本浩史、江原正博（分子科学研究所）：キラル分子におけるスピン軌道相互作用の計算 [4]
3. 山本浩史、岸根順一郎（放送大学）：キラル磁性伝導体の電子状態計算 [1]
4. 山本浩史、Supawadee Namuangruk（NANOTEC, Thailand）機能性分子の電気双極子計算 [5]

(7) Hosted seminars and symposiums

1. 「有機デバイスを用いた量子状態制御の新展開」分子研研究会、岡崎市、2018 年 9 月 29-30 日.
2. 「量子位相に着目した有機デバイスの新展開」第 99 日本化学会春季年会特別企画、京都府、

2019 年 3 月 19 日.

3. “The 80th Okazaki conference –Chirality-induced Spin Selectivity and its related phenomena” (CISS2019), Okazaki, Japan, May 15-18 (2019).
4. 「量子位相化学研究会（QPC2019）」分子研研究会、岡崎市、2020 年 8 月 5-6 日.
5. “In-field Molecules for Next-generations Flexible Electronics”, Cluster G-1, MRM2019, Yokohama, Japan, Dec. 13 (2019).

(8) Awards and honors

1. 須田理行：“文部科学大臣表彰・若手科学者賞”、文部科学省、2018 年 4 月 10 日.
2. 山本浩史：“学術賞”、日本化学会、2019 年 3 月 17 日.
3. 山本浩史：“永井科学技術財団学術賞”、永井科学技術財団、2020 年 3 月 3 日.

(9) Press releases

1. プレスリリース、“有機超伝導体における光の増幅現象を発見　レーザーの原理で超伝導の機構を解明する”、2018 年 6 月 26 日.
   https://www.tohoku.ac.jp/japanese/2018/06/press20180626-02.html
2. プレスリリース、“有機トランジスタで超伝導の条件を探る　ー電圧とひずみで試料の超伝導を制御ー”、2019 年 5 月 13 日.
   https://www.riken.jp/press/2019/20190511_1/
3. プレスリリース、“キラル分子モーターを利用した電子スピンの光・熱による制御”、2019 年 6 月 7 日.
   https://www.ims.ac.jp/news/2019/06/07_4366.html
4. 日経産業新聞、“光や熱で電子スピン制御”、2019 年 6 月 21 日.
5. 科学新聞、“キラル分子モーターの回転運動利用”、2019 年 6 月 28 日.

Curriculum Vita of PI

Name **Affiliation** **Address** **Phone number** **Email**	Hiroyuki Noumi Professor Osaka University, Research Center for Nuclear Physics 10-1 Mihogaka Ibaraki Osaka 567-0047 JAPAN +81-(0)6-6879-8933 noumi@rcnp.osaka-u.ac.jp 
Education	1984-1990 Graduate School of Science, Osaka University 1981-1984 Faculty of Science, Physics Department, Osaka University
Degrees	Dr. Sci. (1991) Osaka University M. Sci. (1987) Osaka University B. Sci. (1985) Osaka University
Employment/research experience	2007- Professor, Research Center for Nuclear Physics, Osaka University 2002-2007 Associate Professor, Institute of Particle and Nuclear Studies (IPNS), High Energy Accelerator Research Organization (KEK) 1997-2002 Research Associate, IPNS, KEK 1990-1997 Research Associate, National Laboratory for High Energy Physics (KEK) <u>Additional post</u> 2019- Visiting Chief Researcher, RIKEN 2018- Professor, Sokendai 2016- Specially Appointed Professor, IPNS, KEK 2013-2019 Visiting Researcher, RIKEN 2013-2016 Visiting Professor, INPS, KEK 2010-2013 Visiting Researcher, RIKEN 2010-2011 Visiting Professor, INPS, KEK 2008-2008 Visiting Researcher, INPS, KEK 2004-2007 Associate Professor, Sokendai 1999-2002 Researcher, Sokendai
Awards and honors	Osaka University Presidential Awards for Achievement (2013) Atomic Energy Society of Japan, North Kanto Branch Awards for Distinguished Service (2005)
Academic activities	Member; Physical Society of Japan (JPS) Chair of Division of Experimental Nuclear Physics, JPS (2019) Deputy Chair of Division of Experimental Nuclear Physics, JPS (2018) Executive Committee Member, Hadron User's Association (2008-2010, 2012-2018, 2020)

	Executive Committee Member, Chair, Hadron User's Association (2016,2017) Executive Committee Member, Deputy Chair, Hadron User's Association (2015) International Advisory Committee Member, International Conference on Hypernuclear and Strange Particle Physics (2015-)

(1) Participants

野海　博之	教授	(核物理研究センター)
白鳥　昂太郎	助教	(核物理研究センター)
小沢　恭一郎	招へい准教授	(高エネルギー加速器研究機構)
冨田　夏希	特任研究員	(核物理研究センター)
井上　謙太郎	特任研究員	(核物理研究センター)
川﨑　新吾	教務補佐員	(核物理研究センター)
Zhadyra Omar	大学院生	(核物理研究センター)
赤石　貴也	大学院生，協同研究員	(大阪大学大学院理学研究科)
Wen-Chen Chang	協同研究員	(Academia Sinica)
永井　慧	協同研究員	(Academia Sinica)
馬　越	協同研究員	(理化学研究所)
浅野　秀光	協同研究員	(理化学研究所)
高橋　智則	協同研究員	(理化学研究所)
本多　良太郎	協同研究員	(東北大学大学院理学研究科)
大西　宏明	協同研究員	(東北大学電子光理学研究センター)
石川　貴嗣	協同研究員	(東北大学電子光理学研究センター)
五十嵐　洋一	協同研究員	(高エネルギー加速器研究機構)
小松　雄哉	協同研究員	(高エネルギー加速器研究機構)

(2) Original papers（Research Category in [ ]）

1. H. Nagahiro, S. Yasui, A. Hosaka, M. Oka, and H. Noumi, “Structure of charmed Baryons studied by pionic decays”, Phys. Rev. **D95**, 014023(2017). [2,1]
2. H. Noumi, “Physics in J-PARC Hadron-Hall Extension”, JPS Conf. Proc. **13**, 010017(2017). [2,1]
3. S. Kawasaki *et al.*, "Spectroscopic Experiment of Λ(1405) via the In-flight d(K−,n) Reaction at J-PARC K1.8BR", JPS Conf. Proc. **13**, 020018(2017). [1]
4. T.N. Takahashi for the J-PARC E50 collaboration, “Experimental Investigation for Diquark Degrees of Freedom in a Charmed Baryon at J-PARC”, JPS Conf. Proc. **13**, 020042(2017). [2,1]
5. K. Inoue *et al.*, "Spectroscopic Study of Hyperon Resonance Below K-N Threshold via the d(K−,n) Reaction", JPS Conf. Proc. **17**, 072003(2017). [1]
6. H. Noumi, “Strange and Charm Hadron Physics at J-PARC in Future”, JPS Conf. Proc. **17**, 111003(2017). [2,1]
7. S. Ajimura et al., ""K-pp", a Kbar-meson nuclear bound state, observed in ^{3}He(K-, Λp)n reactions", Phys. Lett. B **789**, 620-625 (2019). [1]
8. Y. Komatsu *et al*., "Experimental Study of Di-quark Correlation by Charmed Baryon Spectroscopy at J-PARC High-Momentum Secondary Beam Line", JPS Conf. Proc. **26**, 022029 (2019). [2,1]
9. S. Kawasaki *et al*., "Λ(1405)Spectroscopy via the In-flight d(**K**-,n) Reaction at the J-PARC K1.8BR", JPS Conf. Proc. **26**, 022009 (2019). [1,2]

(3) Reviews and books（ Research Category in [ ] ）

1. 岩崎雅彦、野海博之, クォークと反クォークが共存する原子核：K 中間子原子核の世界, パリティ、2019 年 1 月号（Vol2019,No01） 第 34 巻第 1 号 p44-45 [1]

(4) Invited presentations（ Research Category in [ ] ）

1. H. Noumi: “Status E31 – open questions”, “SMI Mini-Workshop on “Future opportunities toward studies in low-energy hadron physics with strangeness”, Stephan Meyer Institute, Vienna, Austria, 3-5 December, 2018 [1,2]
2. H. Noumi: “Future Experiment at J-PARC”, “SMI Mini-Workshop on “Future opportunities toward studies in low-energy hadron physics with strangeness”, Stephan Meyer Institute, Vienna, Austria, 3-5 December, 2018 [1,2]
3. H. Noumi: “E50 High-momentum beamline”, 52nd Reimei Workshop on “Experimental and Theoretical Hadron Physics: Recent Exciting Developments”, IQBRC, Tokai, 9-11

January, 2019 [2,1]

4. H. Noumi: "Hadron physics with hadron beams at J-PARC", "Korea-Japan Joint Workshop on the Present and the Future in Hadron Physics at J-PARC", Pukyong National University, Busan, Korea, 4-5 March, 2019. [1,2]
5. H. Noumi: "Experimental study of Lambda(1405) resonance via kaon-induced reactions on deuteron", 3rd Jagiellonian Symposium on Fundamental and Applied Subatomic Physics, Collegium Maius, Krakow, Poland, 23-28 June 2019. [1,2]
6. 野海博之: "J-PARC 高運動量ビームで探るハドロンの内部構造", "日本物理学会 2019 年秋季大会 実験核・素実・理論核合同セッション　高エネルギーQCD・核子構造"(企画講演), 山形大学, 17 Sep, 2019. [2,1]
7. K. Shirotori: "Hadron spectroscopy with high-momentum hadron beams", The 3rd J-PARC symposium (J-PARC2019), Tsukuba, 24-26 September 2019 [2,1]
8. H. Noumi: "Production of charmed baryons at J-PARC", XVth RECONTRES du VIETNAM "Perspectives in Hadron Physics", ICISE, Quy Nhon, Vietnam, 22-28 September, 2019. [2,1]
9. 白鳥昂太郎："Spectroscopy experiment of multi-strangeness baryons at the J-PARC high-momentum beam line"，ELPH 研究会 C024「ハドロン構造における多粒子相関」，東北大学電子光理学研究センター，2019 年 10 月 16 日- 10 月 17 日［2, 1］
10. H. Noumi: "High-momentum pion beamline at J-PARC and Open Charm Production", "Reimei Symposium on Synergies in Hadron Physics between J-PARC and JLab", Jefferson Lab., Virginia, USA, 5 November, 2020. [2,1]
11. H. Noumi: "Result of the J-PARC E31 experiment", "Workshop on Physics of Heavy-quark and Exotic Hadrons", Tokai, J-PARC, 27-29 January, 2020. [1,2]
12. H. Noumi: "Hadron physics at the J-PARC high-momentum beam line", "Workshop on Physics of Heavy-quark and Exotic Hadrons", Tokai, J-PARC, 27-29 January, 2020. [2,1]

(5) Patent applications（ Research Category in [ ] ）

N/A

(6) Collaborations including both inside and outside project（ Research Category in [ ] ）

1. 白鳥昂太郎、冨田夏希、野海博之、浅野秀光（理研）、馬越（理研）、佐久間史典（理研）、山我拓巳（理研）、Wen Chen Chang(台湾中央研究院)、Roger Wendell(京都大学)、Akira Konaka(TRIUMF)ほか EMPHATIC Collaboration: ニュートリノフラックス精度向上のためのハドロンの散乱と生成断面積測定 [1]
2. Sang-In Shim（大阪大学)、保坂淳（大阪大学)、Hyun-Chul Kim（仁荷大学)、野海博之：チャームバリオン生成反応に関する理論研究 [2,1]
3. 永廣秀子（奈良女子大学)、安井繁宏（東工大)、保坂淳（大阪大学)、岡真（東工大)、野海博之：チャームバリオンの構造とπ放出崩壊幅に関する理論研究 [2,1]

(7) Hosted seminars and symposiums

1. RCNP 研究会 "Physics with General Purpose Spectrometer in the High-momentum Beam Line", Osaka, Japan, August 27-28 (2018).
2. "Secrets of PRL", Prof. Robert Garisto (American Physical Society), SEP 19th, 2018
3. Workshop on hadron physics with heavy quarks, RCNP, Jan 21, 2020

(8) Awards and honors

1. Zhadyra Omar："ANPhA 3rd Prize"、SNP School 2018、2017 年 8 月 3 日.
2. 赤石 貴也："修士論文賞"、ハドロンホールユーザー会、2019 年 3 月 14 日
3. Zhadyra Omar："ANPhA 1st Prize"、SNP School 2019、2019 年 9 月 8 日.
4. Zhadyra Omar："橋本賞"、SNP School 2019、2019 年 9 月 8 日.

(9) Press releases

1. K-中間子と二つの陽子からなる原子核の発見 -クォークと反クォークが共存する"奇妙な"結

合状態-, 理化学研究所、 高エネルギー加速器研究機構、 日本原子力研究開発機構、 大阪大学、 東北大学、 Istituto Nazionale di Fisica Nucleare、The Stefan Meyer Institute、J-PARC センター, 2019 年 1 月 24 日 [1]
https://www.riken.jp/press/2019/20190124_2/index.html