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RIKEN SPring-8 Center

SPring-8 to sustainable future



SPring-8
to sustainable future



Preface

The publication of the ‘Spring-8 official guidebook’ in 2017 helped celebrate the twentieth anniversary of Spring-8's opening. That booklet provided easy-to-understand explanations of typical use cases for each of our beamlines. Its unexpected popularity forced us to republish new editions because many universities and other learning institutions used it as lecture material over the last few years.

We decided to update the booklet to categorize Spring-8 use cases according to the Sustainable Development Goals (SDGs) adopted at the 2015 United Nations Summit. The seventeen SDGs are to be accomplished by 2030 to achieve a sustainable and diverse society.

This booklet showcases the capabilities of Spring-8 by associating the specific results of work at Spring-8 with each of the SDGs: what types of use cases are applicable, which beamlines are appropriate, and what are the achievable outcomes. We sincerely hope that Spring-8 can enable progress to address the many challenges that have yet to be confronted effectively.

We have edited this booklet in order to help junior-high and high-school students understand leading-edge science, since they will be responsible for the future. We hope that our diverse audience finds this booklet useful!

A handwritten signature in blue ink, likely belonging to the Director of the RIKEN Spring-8 Center.

Director
RIKEN Spring-8 Center



Preface

SPRING-8's activities supporting the SDGs

Research by Topic

- Materials
- Information Technology and Devices
- Energy and Environment
- Fundamental Materials Science
- Geophysics and Astronomy
- Medical Science
- Fundamental Biology
- Food, Life and Society

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Research Activities

Synchrotron Facilities around the World

Introduction to X-rays

SPRING-8

Beamline Map

SACLA

SPRING-8 and SACLA in the Future



SPRING-8's activities supporting the SDGs



ELIMINATION OF POVERTY

Contributes to the development of materials and devices that enable people to connect with each other and work anywhere around the world



ZERO HUNGER

Clarifies how our body takes in nutrients, and contributes to the development of functional foods



GOOD HEALTH AND WELL-BEING

Clarifies the structures and functions of proteins applicable for pharmaceutical research and combating disease



QUALITY EDUCATION

Addresses current problems, and describes them in common language that anyone can understand



GENDER EQUALITY

Reduces gender discrepancies by advancing and popularizing science



CLEAN WATER AND SANITATION

Reveals the mechanisms causing various types of pollution



AFFORDABLE AND CLEAN ENERGY

Contributes to the development of energy-saving and compact devices



DECENT WORK AND ECONOMIC GROWTH

Develops technology that promotes efficient production



INDUSTRY, INNOVATION AND INFRASTRUCTURE

Explores new materials and phenomena, and provides guidelines for industrial applications



REDUCED INEQUALITY

Contributes to the creation of materials and devices for all people, anywhere in the world



SUSTAINABLE CITIES AND COMMUNITIES

Contributes to the development of robust, light and restorable housing materials



RESPONSIBLE CONSUMPTION AND PRODUCTION

Investigates the destruction mechanisms of materials and provides guidelines for incorporating the eventual breakdown of materials in their designs



CLIMATE ACTION

Investigates how the states of materials change depending on temperature and humidity, and contributes to the development of disaster-resistant materials



LIFE BELOW WATER

Researches the effects of marine pollution on materials



LIFE ON LAND

Clarifies the mechanisms of photosynthesis, discovers techniques for artificial photosynthesis, and contributes to forest protection



PEACE, JUSTICE AND STRONG INSTITUTIONS

Contributes to forensic investigations



PARTNERSHIPS FOR GOALS

Promotes scientific research in collaboration with synchrotron facilities around the world

Materials

- P 1-1 Improving the durability of stainless steel
- P 2-1 Developing stronger and more durable aluminum materials
- P 3-1 New approach for developing functional materials
- P 4-1 Highly-durable luminescent materials
- P 5-1 Production of innovative glass materials
- P 6-1 New material made of tough polymers for the bodies of electric vehicles
- P 7-1 Development of catalysts
- P 8-1 Hydrogen storage using aluminum-based materials
- P 9-1 High-performance nitride semiconductors for photovoltaics
- P10-1 Improving the properties and capabilities of steel
- P11-1 Improving the mechanical reliability of ceramics
- P12-1 Radical enzymes for industrial use
- P13-1 Super-tough materials for ceramics
- P14-1 Deeper understanding of laser processing of light materials
- P15-1 Understanding and designing functional materials
- P16-1 Design for structural materials with lightness and hardness
- P17-1 Making stronger magnets with new uses
- P18-1 Discovering the source of strength and durability of bagworm silk
- P19-1 Tougher silk materials with synthetic peptides
- P20-1 Design of material destruction
- P 1-2 Materials that have zero thermal-expansion ability
- P 2-2 Nano-alloy design with new functions
- P 3-2 Toward effective use of light element materials
- P 4-2 Fabrication of a new type of functional glass
- P 5-2 Controlling durability and flexibility at the molecular level
- P 6-2 Development of surface-controlled steel with high corrosion resistance
- P 7-2 Development of materials for building more resilient infrastructure
- P 8-2 Elucidating the electronic states in innovative hybrid materials
- P 9-2 Development of a tungsten recycling process
- P10-2 Preventing aluminum degradation
- P11-2 Development of tires with greater fuel efficiency
- P12-2 New nanotubes with periodic vacancy defects
- P13-2 New optical and electronic materials
- P14-2 Improvement of fluorite lens performance
- P15-2 Creation of new functional materials
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Information Technology and Devices

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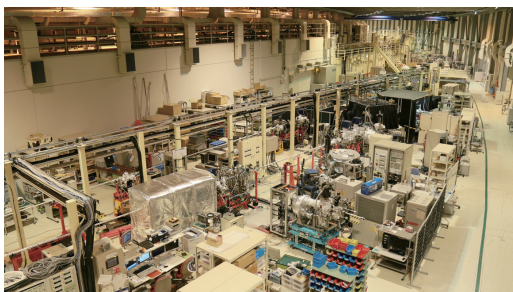


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Food, Life and Society

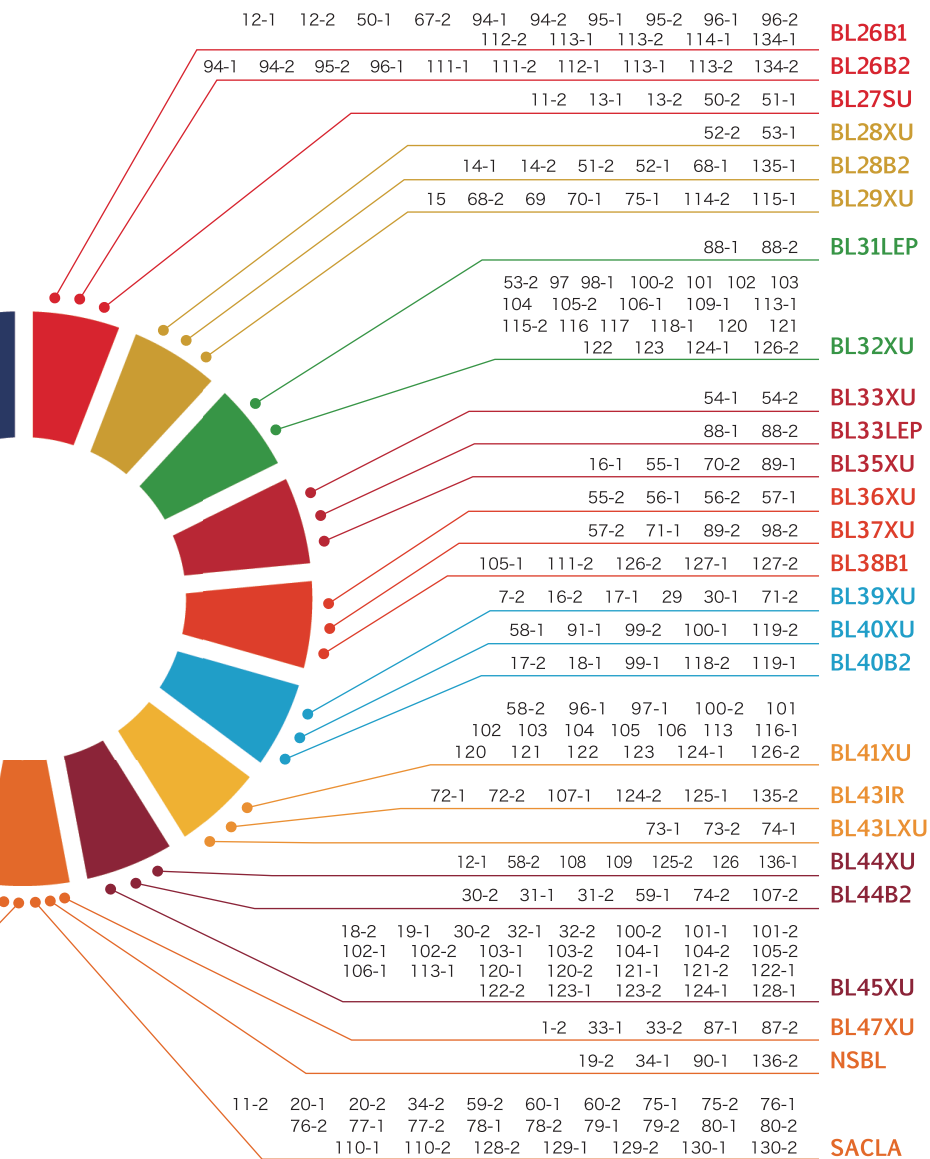
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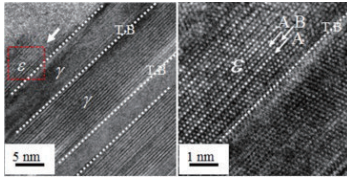
BL01B1	5-1 35-1 35-2 131-1
BL02B1	1-1 3-1 21-1 21-2 22-1 91-1 134-2
BL02B2	1-2 2-1 2-2 3-2 4-1 21-1 36-1 36-2 37-1 39-1 61-1 64-2 91-2 131-2 134-2
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BL22XU	1-2
BL24XU	67-1 133-1 133-2
BL25SU	26-2 27-1 27-2 28-1 28-2 29-1 29-2 49-2



Improving the durability of stainless steel

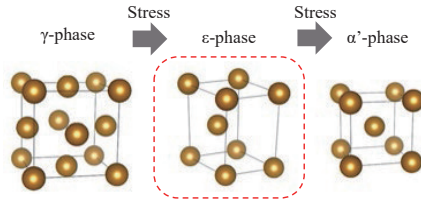
- Applying stress to stainless steel and observing the appearance of new phases at the nanoscale level
- Controlling the strength and durability of stainless steel without relying on empirical rules

Photo of stainless steel electron microscope



Some phases are recognizable but only the surface is known.

Structural change of each phase transformed by stress during processing



We discovered the existence of this mesophase!

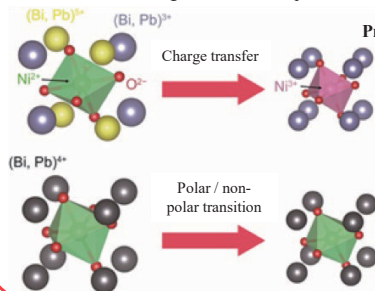


Reference: M. Hatano *et al.*, *Phil. Mag. Lett.*, **96**, 220 (2016)

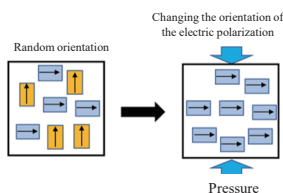
Materials that have zero thermal-expansion ability

- Developing materials with negative thermal-expansion properties after identifying the source of this capability to be charge transfers and polarization changes during heating
- Finding materials that can control dielectric polarization capabilities
- Incorporating these materials in new devices, such as optical communications and semiconductor manufacturing equipment

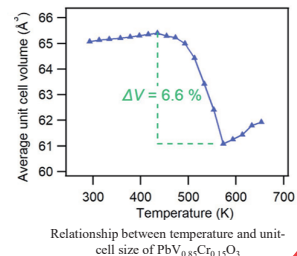
Mechanism of the negative thermal expansion



Pressure effect on electric polarization



Negative thermal expansion

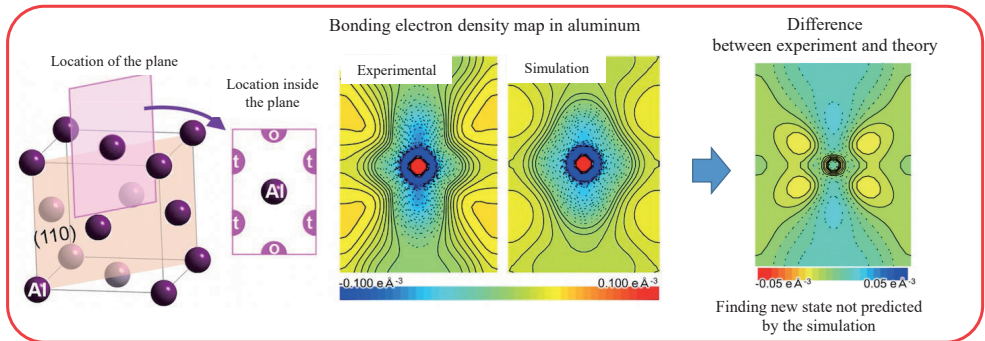


Relationship between temperature and unit-cell size of $\text{PbV}_{0.85}\text{Cr}_{0.15}\text{O}_3$



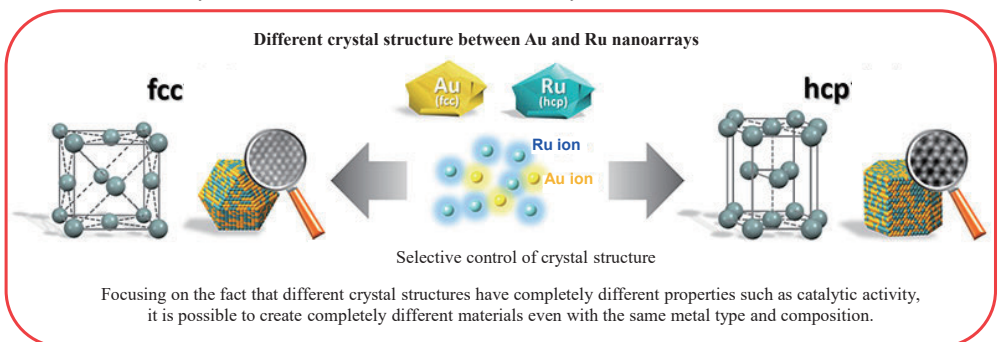
Reference: Y. Sakai *et al.*, *Chem. Mater.*, **31**, 13, 4748 (2019)
T. Ogata *et al.*, *Chem. Mater.*, **31**, 4, 1352(2019)

- Developing stronger and more durable aluminum materials
 - Observing a new chemical bonding state in aluminum
 - Providing helpful guidelines for improving the functionality of aluminum by elucidating the direction dependence of Young's modulus and the origin of mechanical properties such as shear strength



Reference: T. Sasaki *et al.*, *Sci. Rep.*, **8**, 11964 (2018)

- Nano-alloy design with new functions
 - Created gold and ruthenium nano-alloys with different crystal structures from the same composition
 - Proposed a new method for controlling the crystal structures of nano-alloy materials
 - Developing new magnetic materials, catalysts, and optical materials using innovative crystal structure control methods for nano-alloys

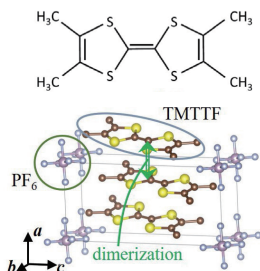


Reference: Q. Zhang *et al.*, *Nat. Commun.*, **9**, 510 (2018)

New approach for developing functional materials

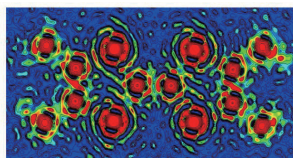
- Developed a method for visualizing molecular orbital distribution using precise structural analysis
- Succeeded in directly observing valence electron distribution and clarified the forty-year mystery of "transitions without structural change"
- Designing materials based on molecular orbital information

Molecular structure of TMTTF



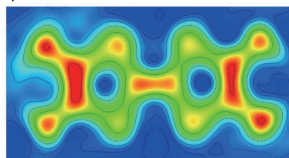
Proposal of electron density analysis method by core difference Fourier synthesis (CDFS) method

Conventional method


 $0 \text{ e}/\text{\AA}^3$

Fake electron density around atoms is estimated.

CDFS method


 $1.8 \text{ e}/\text{\AA}^3$

Molecular orbitals were clearly observed.

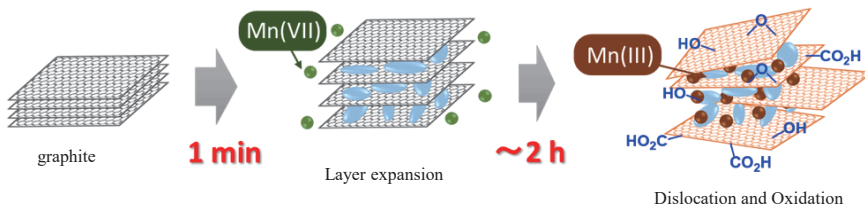


Reference: S. Kitou *et al.*, *Phys. Rev. Lett.* **119**, 065701 (2017)

Toward effective use of light element materials

- Observed *in situ* the reaction process of synthesizing graphene oxide from graphite
- Found a suitable reaction time and oxidizing agent for synthesizing graphene oxide
- Providing a synthesis procedure for graphene oxide

Structural evolution from graphite to graphene oxide



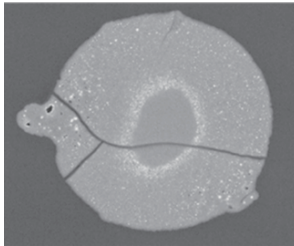
Promising material for improving performance such as electrode, catalysts, lubricants, and heat conductive materials.



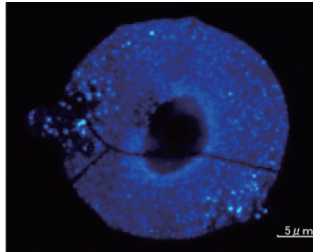
Reference: N. Morimoto *et al.*, *Chem. Mater.*, **29**, 2150 (2017)

- Highly-durable luminescent materials
 - Synthesizing "nano-composite phosphor" with excellent durability and high luminous performance
 - Providing clues for understanding the formation mechanisms
- Expanding potential candidates for developing better luminescent materials

Cross-sectional SEM image of nanocomposite phosphor



Emission image by electron beam irradiation



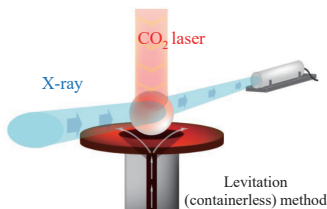
Only 2% decrease in emission intensity observed after exposure of phosphor for 2000 hours at high temperature (85 °C) and high humidity (85%)



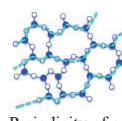
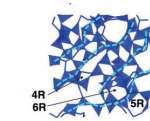
Reference: H. Daicho *et al.*, *ACS Appl. Mater. Interfaces*, **9**, 41405 (2017)

- Fabrication of a new type of functional glass
 - Holding a liquid at a high melting point (2715 °C) in the air using a levitation method
 - Elucidating the differences in structure at the nanoscale level between glass-forming and non-glass-forming liquids
- Developing ultra-high refractive index glass and new types of ceramics

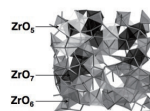
Glass is synthesized by quenching liquid, but some liquids do not turn into glass



Levitation method is useful for probing the structure of high-temperature liquid over 2000 °C



Periodicity of cage boundaries



No obvious periodicity

Glass-forming liquid
(e.g. silica)

Non-glass-forming liquid
(e.g. zirconia)

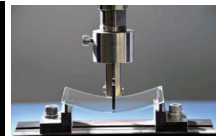
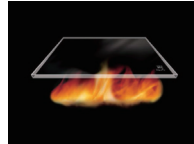
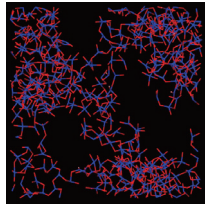
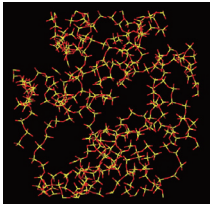


Reference: S. Kohara *et al.*, *Nat. Commun.*, **5**, 5892 (2014)

Production of innovative glass materials

- Observed the atomic arrangement in glass with a disordered structure
- Discovered the relationship between the heat-resistance property of glass and the changes in network structure
- Developing more heat-resistant glass

Modification in network structure due to changes in glass composition



Development of new glass materials

Thermal expansion is very sensitive to the substitution of the network former.

Images are provided by AGC

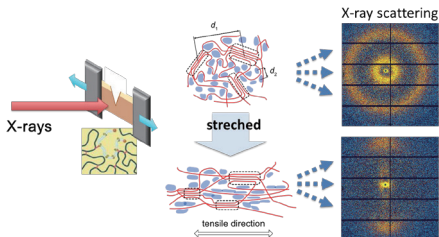


Reference: Y. Onodera *et al.*, *Nat. Commun.*, **8**, 15549 (2017)

Controlling durability and flexibility at the molecular level

- Investigated fracture phenomena in polymer materials
- Making plastic products more durable

X-ray scattering by the polymer chains changes when the polymer materials are deformed.



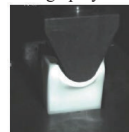
By examining the arrangement of molecules, the mechanism of fracture can be understood.

Impact-resistant plastics

Conventional



Tough polymer



(provided by TORAY)



Materials

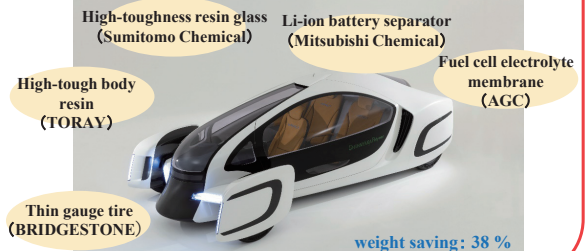
BL05XU

- New material made of tough polymers for the bodies of electric vehicles
 - Developed polymer materials that are both flexible and durable for use in electric vehicles
 - Making materials for not only vehicles, but consumer goods such as sports equipment, PC housing, strollers, wheelchairs, etc.

High performance polymer materials

Light Energy Saving
Hard Ductile
Safety Self-Healing

Concept car made of tough polymers

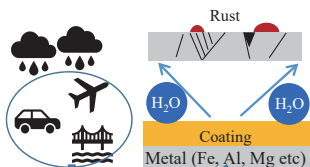


Materials

BL08B2

- Development of surface-controlled steel with high corrosion resistance
 - Elucidation of the rust phenomena of metal surfaces using synchrotron radiation, machine learning, and mathematical analysis technologies
 - Predicting product lifespan and the time required for deterioration, and making society safer through better design of various safety products

Deterioration of social infrastructure mainly caused by the rust of steel

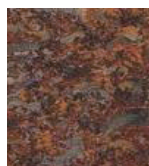


With regards to development of the corrosion resistance steel and coating, it is important to elucidate the chemical changes occurring on metal surfaces and material interfaces.

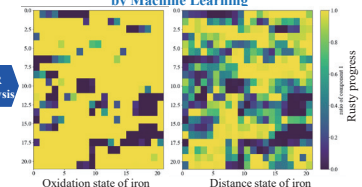
Analytical approaches by applying Machine Learning and mathematical analysis technologies to build a mathematical model to explain rust progress at metal surfaces

Detailed visualization of rust distribution by Machine Learning

Rusted surface



SR analysis



Evaluation of rust progress on metal surfaces makes great progress.

One step towards elucidating the rust phenomenon



Development of catalysts

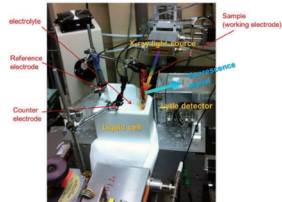
- Control chemical reactions using catalytic nano-particles
- Study the role of nano-catalysts under functioning conditions
→ Developing fuel cell devices and carbon cycle devices

Catalysis
Control chemical reaction



Understand the role of catalyst by X-ray studies

Improvement of catalysis



In situ X-ray Absorption@BL12B2



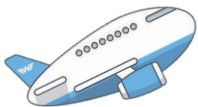
Reference:

J.Gu, *et al.*, *Science*, **364**,1091 (2019)
H. B. Yang *et al.*, *Nat. Energy*, **3**, 140 (2018)

Development of materials for building more resilient infrastructure

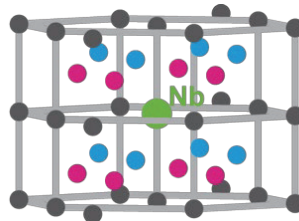
- Investigated characteristic changes of titanium alloys using Nb doping
- Revealed why machining alloys becomes easier using Nb doping
→ Designing materials at the atomic scale with specified properties

Titanium alloys have comparable strength but lighter half than steel.



A wide variety of applications such as aircraft materials, glass frame, and artificial bone

ω -Ti phase surrounding a Nb atom

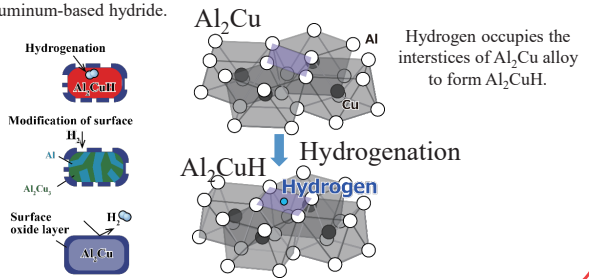
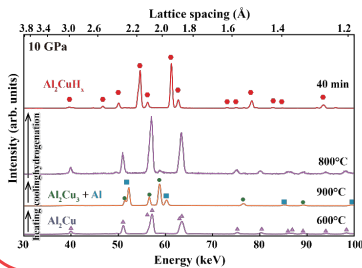


Reference: Yamamoto *et al.*, *Acta Mater.*, **131**, 534 (2017)

Hydrogen storage using aluminum-based materials

- Created an aluminum-based hydride that was impractical for synthesis
- Manufacturing lightweight hydrogen storage alloys

Synchrotron radiation x-ray in-situ observation and high-pressure hydrogen enable us to find synthesis conditions of a novel aluminum-based hydride.

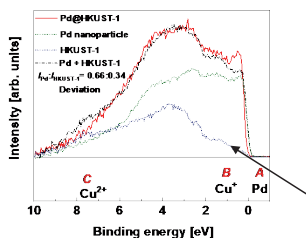


Reference: H. Saitoh *et al.*, *APL Mater.*, **1**, 032113 (2013)

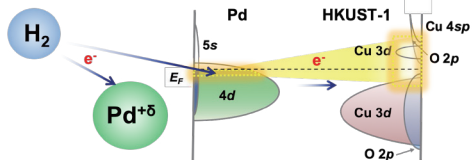
Elucidating the electronic states in innovative hybrid materials

- Investigated the electronic states of a hybrid hydrogen storage material composed of Pd nanocubes
- Discovered the charge transfer from the Pd nano-cubes to the MOFs
- Creating high hydrogen storage capacity for these hybrid materials

HAXPES Valence band spectra reflects electronic state near Fermi level



Schematic illustration for the change of electronic structures at the composite interface corresponding to the charge transfer process and the hydrogen absorption



Deviation (shown in cyan in the left figure) confirmed the charge transfer between two bands above.

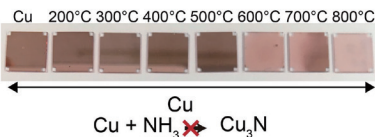


Reference: Y. Chen *et al.*, *Comm. Chem.*, **1**, 61 (2018)

High-performance nitride semiconductors for photovoltaics

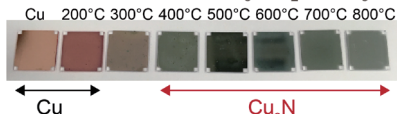
- Fabricated a high-mobility copper nitride acting as an *n*-type semiconductor with *p*-type conduction provided by fluorine doping
- Revealed the electronic properties using synchrotron radiation X-rays
- Developing a unique nitriding technique suitable for mass production

NH_3 gas atmosphere



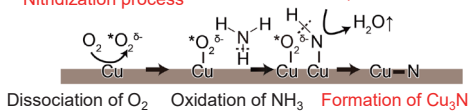
- ✓ Nitridization does not occur
- ✓ Cu is always a metal

Direct nitriding $\text{Cu} + \text{NH}_3 / \text{O}_2 \rightarrow \text{Cu}_3\text{N}$



Nitridization process

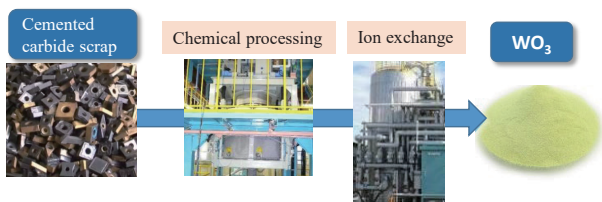
(Semiconductor)



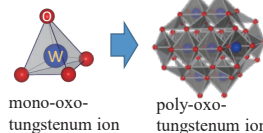
Reference: K. Matsuzaki *et al.*, *Adv. Funct. Mater.* **30**, 1801968 (2018)

Development of a tungsten recycling process

- Optimized the ion exchange process
- Developed a highly efficient recycling process
- Shortening the development period for recycling



For high efficiency of the ion exchange, the process conditions were optimized for using poly-oxo-tungsten ion in stead of mono-oxo-tungsten ion



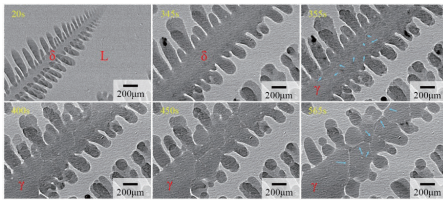
SUNBEAM•Sumitomo Electric Industries, Ltd.

Reference: J.Iihara, *JSSRR*, **27**, 253 (2014)

Improving the properties and capabilities of steel

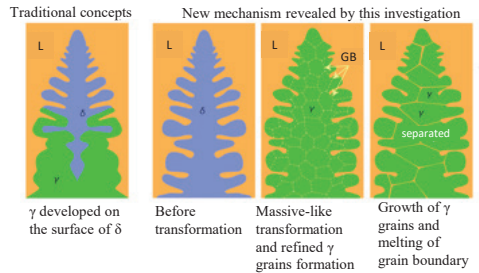
- During the steel solidification process, refined γ grains were produced simultaneously with massive-like δ - γ transformation.
 - The fragmentation of a dendrite was induced by melting at the γ grain boundary and δ - γ interface.
- Controlling microstructures that determine the strength of a material via direct observation

X-ray imaging of the steel solidification



δ dendrite and γ grains occurred in the dendrite

Massive-like transformation and formation of γ grains

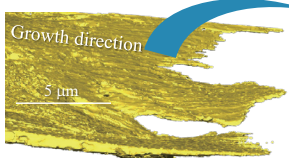


Reference: H. Yasuda *et al.*, *Nat. Commun.*, **10**, 3183 (2019)

Preventing aluminum degradation

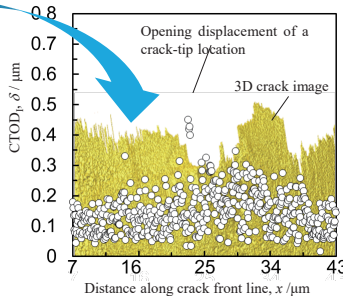
- Revealed the singular fracture behavior of high-strength aluminum using 4D (3D + time) observation
 - Found a propagating crack with a sharp crack-tip accompanied by sufficient plastic deformation
- Proposing prevention methods and clarifications for environmentally-assisted cracking and hydrogen embrittlement (HE), examined in terms of fracture micro-mechanisms

3D intergranular crack image

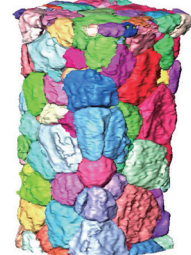


A crack caused by HE (Upper figure) and corresponding crack-tip opening displacement (CTOD) distribution along a crack front line (Right figure), implying extraordinarily sharp crack of 0.1 μm in CTOD is characteristic

Crack-tip opening profile



3D image of a polycrystal



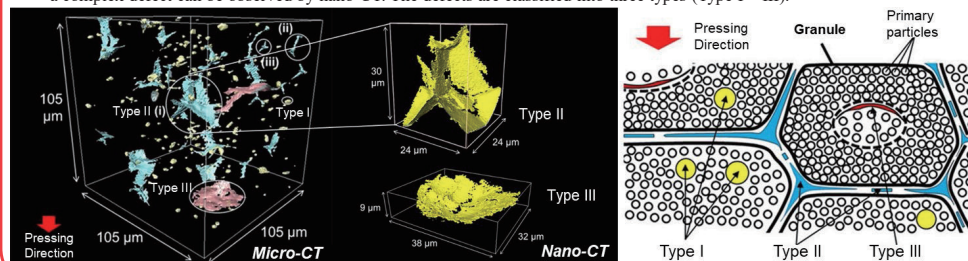
Assessment of crack-microstructure relationships during HE



Reference: H. Su, H. Toda *et al.*, *Acta Materialia*, **159**, 332 (2018)
H. Su, H. Toda *et al.*, *Acta Materialia*, **176**, 96 (2019)

- Improving the mechanical reliability of ceramics
 - Observed the distribution and 3D morphology of defects in ceramics
 - Estimated fracture strength based on defect sizes, shapes, orientations, and distribution
- Controlling internal defects formed during powder processing to improve mechanical reliability

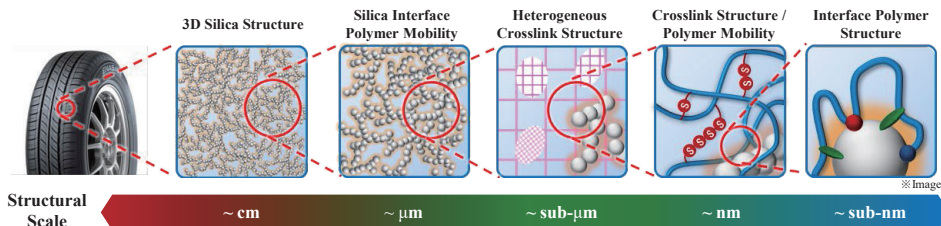
Micro-CT reveals the distribution of large strength-limiting defects in the entire body of a sample, while the detailed shape of a complex defect can be observed by nano-CT. The defects are classified into three types (Type I ~ III).



Reference: G. Okuma *et al.*, *Sci. Rep.*, **9**, 11595 (2019)

- Development of tires with greater fuel efficiency
 - Produced tires that balanced strong grip with high fuel efficiency after revealing the complex internal structures of rubber
- Demonstrating the usefulness of synchrotron radiation analysis in developing products that represent a great step toward improving both environmental friendliness and performance/functionality

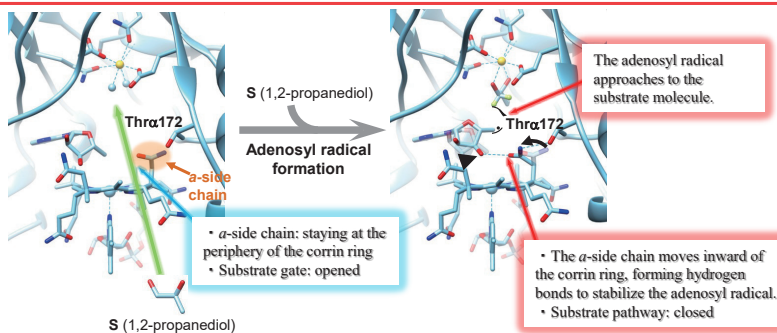
Analyzing the internal state of tire rubber at various scales of magnitude, we developed tires that combine lower friction for greater fuel efficiency when driving with stronger grip for safety when braking.



Sumitomo Rubber Industries, Ltd.

■ Radical enzymes for industrial use

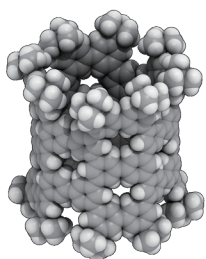
- Analyzed the structures of radical enzymes catalyzing chemically-difficult reactions, complexed with active coenzyme B₁₂
 - Revealed how the active coenzyme controls the radical reactions, avoiding accidental side-reactions in the enzymes
- Producing improved catalytic properties that may lead to useful chemicals derived from low-cost materials that exploit the high reactivity of radical specimens



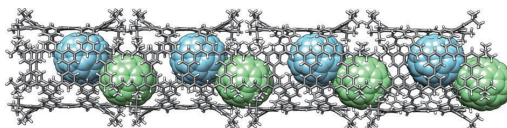
Reference: N. Shibata *et al.*, *Angew. Chem. Int. Ed.*, **57**, 7830 (2018)

■ New nanotubes with periodic vacancy defects

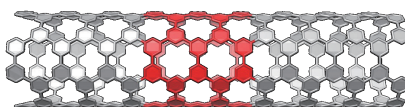
- Synthesized nanotube molecules (phenine nanotube: pNT) with periodic vacancy defects
 - Found forty benzene panels (phenine) linked by three types of coupling reactions
- Creating applications for various fields, such as materials science



Crystal structure of pNT



Packing structure of pNT encapsulating fullerene C₇₀



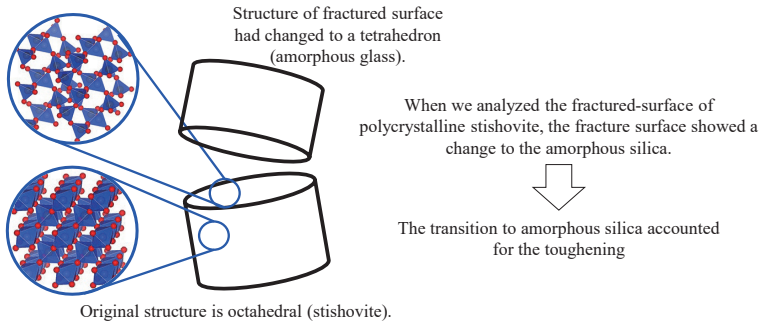
The new pNT molecule is a segment of an infinite nanotube with periodic vacancy defects.



Reference: Z. Sun *et al.*, *Science*, **363**, 151 (2019)

■ Super-tough materials for ceramics

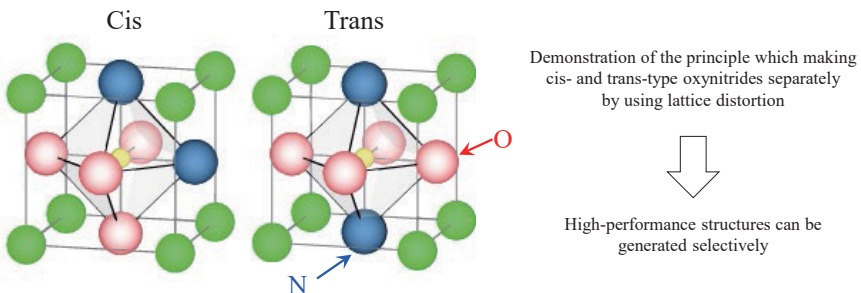
- Investigation of fracture-induced amorphization, providing a new platform to produce more durable ceramics
- Developing super-hard and super-tough ceramics



Reference: N. Nishiyama *et al.*, *Sci. Rep.*, **4**, 6558 (2014)

■ New optical and electronic materials

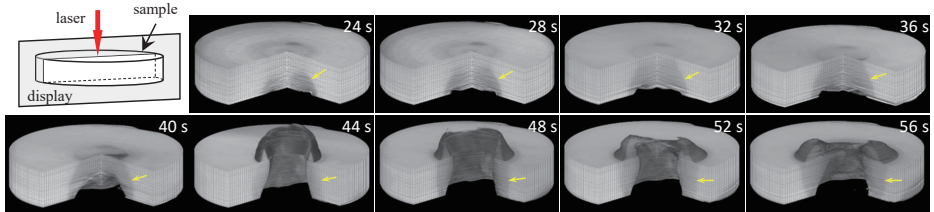
- Demonstration of strain engineering
- Designing new optical and electronic materials



Reference: D. Oka *et al.*, *ACS Nano*, **11**, 4, 3860 (2017)

- Deeper understanding of laser processing of light materials
 - 3D visualization of dynamic changes in polymers and carbon fiber reinforced plastics (CFRP) under laser irradiation
 - Understanding and controlling damage extension deep within materials undergoing laser processing

Phase tomography by X-ray Talbot interferometer with pink beam extracted from white synchrotron radiation

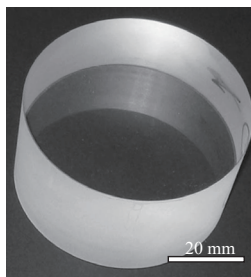


Polypropylene under infrared laser irradiation: expansion of melting zone (yellow arrows) were depicted.



Reference: K. Vegso et al., *Sci. Rep.*, **9**, 7404 (2019)

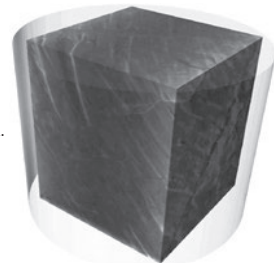
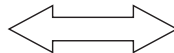
- Improvement of fluorite lens performance
 - Clarified the origin of the non-uniform refractive index distribution that degrades the performance of lenses by using X-ray topography
 - Specifying guidelines for the development of high-performance lenses



Photograph of fluorite lens

Observation of fluorite lens by X-ray topography

Refractive index distribution corresponded to lattice defect distribution.



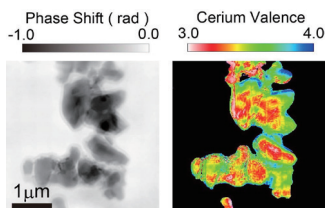
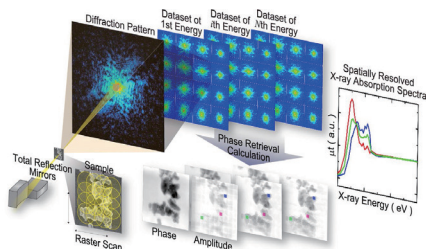
X-ray topographic image of fluorite lens
Bright contrast indicates the distribution of lattice defects.



Reference: Mukaide et al., *JSR*, **13**, 484 (2006)

- Understanding and designing functional materials
 - Visualization of electron density and oxidation state distribution in oxygen storage/release materials
 - Applying nano-structure and chemical state analysis to new functional materials

X-ray spectro-ptychography (ptychographic-XAFS) method



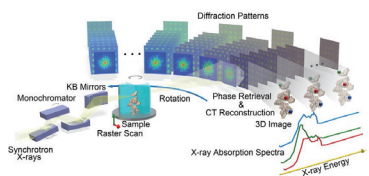
Understanding the relationship between nano-structure and chemical state



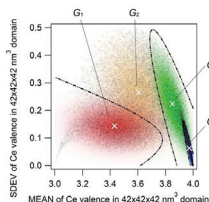
Reference: M. Hirose *et al.*, *Angew. Chem. Int. Ed.*, (2018)

- Creation of new functional materials
 - 3D nano-imaging with unsupervised learning
 - Visualizing the oxidation processes in oxygen storage/release materials
 - Understanding the origin of functions to enable design of innovative materials

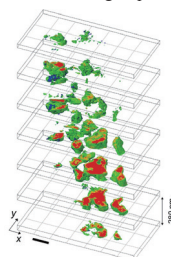
Three-dimensional X-ray spectro-ptychography measurement



Grouping oxygen storage process using unsupervised learning

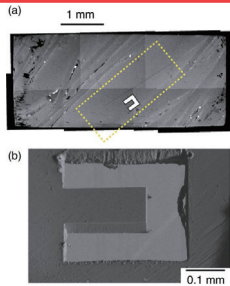


Three-dimensional map of location of groups

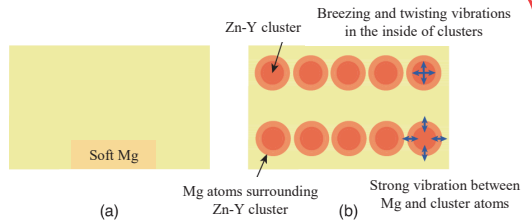


Reference: M. Hirose *et al.*, *Commun. Chem.* **2**, 50 (2019)

- Design for structural materials with lightness and hardness
 - Atomic-scale investigation of the mechanisms in Mg alloys that are hardened by impurity elements
 - Developing guidelines for atomic-scale design for innovative structural materials



Micrograph of hardened Mg alloys precipitated with adding impurity elements

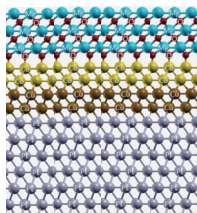


Hardening mechanism of soft Mg alloys assisted by hard impurity clusters

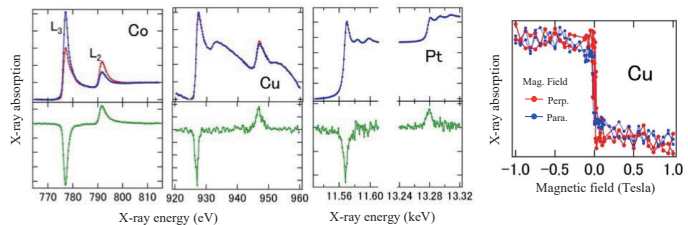


Reference: S. Hosokawa *et al.*, *Acta Materialia*, **146**, 273 (2018)

- Discovering copper magnetism for new types of magnetic devices
 - Observed new magnetic structures in copper (Cu), a non-magnetic element
 - Controlled the magnetic properties by changing the thickness of a Cu thin film
 - Developing a new type of magnetic film with magnetization that is perpendicular to the surface



An atomic structure of the magnetic device studied. Cu atoms are sandwiched by Co and Pt atoms.



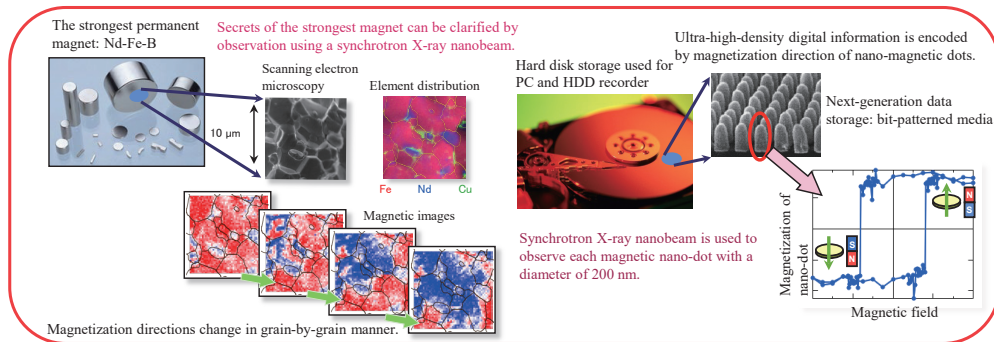
Absorption spectra of circularly polarized X-ray show an evidence of clear magnetic properties of Cu as well as Co and Pt. Cu spin aligned in the direction perpendicular to the film plane.



Reference: J. Okabayashi *et al.*, *Sci. Rep.* **7**, 46132 (2017)

Making stronger magnets with new uses

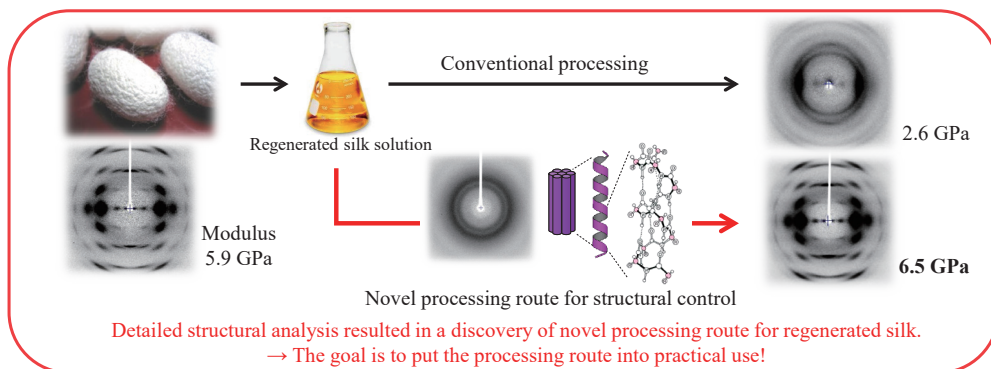
- Observed magnetic materials and artificial devices using a focused beam of 100nm²
- Revealed nano-scale magnetic properties and mechanisms in strong permanent magnets and high-density magnetic data storage
- Developing stronger magnets and new advanced magnetic devices



Reference: M. Suzuki *et al.*, *J. Phys.: Conf. Ser.*, **430**, 012017 (2013)
M. Suzuki *et al.*, *Acta Mat.*, **106**, 155 (2016)

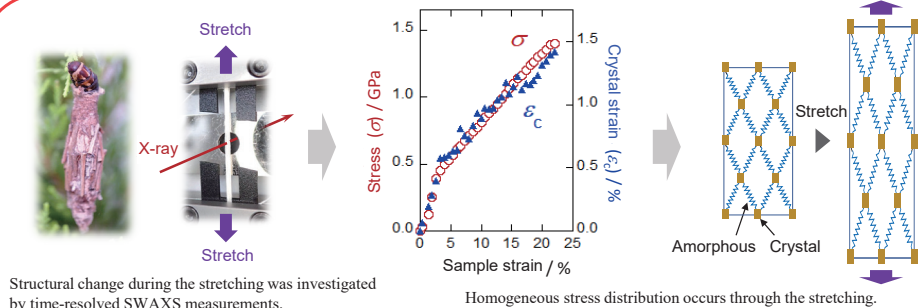
Method for fabricating a regenerated-silk-fiber that is superior to native silk

- Induced an α -helical conformation using HFIP solvent
- Created a hexagonally packed aggregation state of α -helices by self assembly
- Induced the orientation and structural transition (from α -helix to β -sheet) by hot-stretching
- Achieving higher orientation and modulus



Reference: T. Yoshioka *et al.*, *Biomacromolecules*, **17**, 1437 (2016)

- Discovering the source of strength and durability of bagworm silk
 - Determined that bagworm silk has a highly ordered hierarchical structure, which is closely ascribed to its highly-repetitive amino acid sequence
 - Found that the ordered structure transmits tensile stress homogeneously into crystals, and remains unchanged until fibers break
- Designing highly robust artificial threads

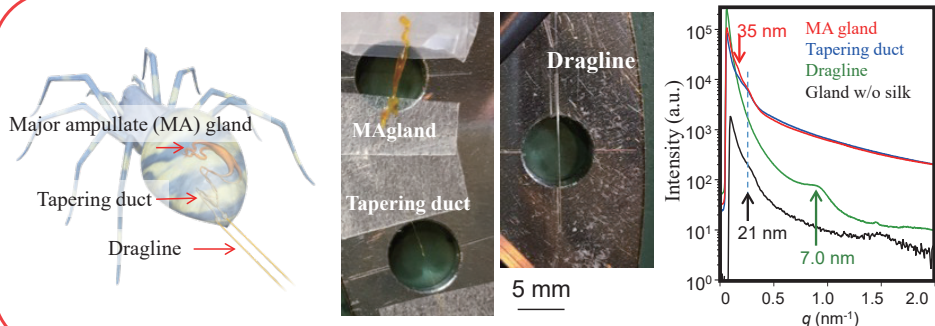


The outstanding mechanical property is the result of a highly ordered hierarchical structure!



Reference: T. Yoshioka *et al.*, *Nat. Commun.*, **10**, 1469 (2019)

- Unique properties of spider draglines
 - Studied the molecular and structural mechanisms underlying the durability of spider draglines
 - Analyzed structural changes during the formation and deformation of draglines
- Contributing to the design and development of innovative materials

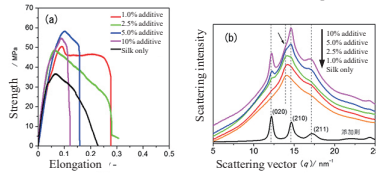
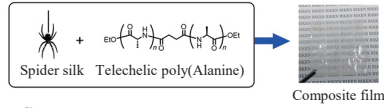
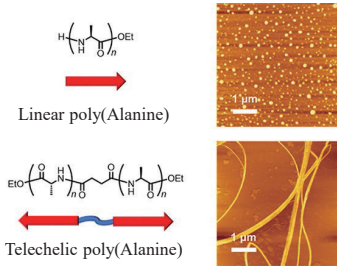


Reference: Yazawa *et al.*, *Commun. Mater.*, **1**, 10 (2020)
 Oktaviani *et al.*, *Chem. Commun.*, **55**, 9761 (2019)
 Yazawa *et al.*, *Macromol. Biosci.*, **18**, 1800220 (2018)
 Oktaviani *et al.*, *Nat. Commun.*, **9**, 2121 (2018)
 Lin *et al.*, *Biomacromolecules*, **18**, 1350 (2017)
 Numata *et al.*, *Soft Matter.*, **11**, 6335 (2015)

Tougher silk materials with synthetic peptides

- Synthetic peptide additives enhanced the mechanical properties of silk materials, triggered by structural changes through measurements
- Creating durable polymeric materials to serve as alternatives to petroleum-based plastics

Chemical structure of synthetic peptides and atomic force microscopy images of their assembly morphologies



Telechelic poly(Alanine) induced appropriate beta-sheet structure formation to improve the mechanical prop of silk materials.

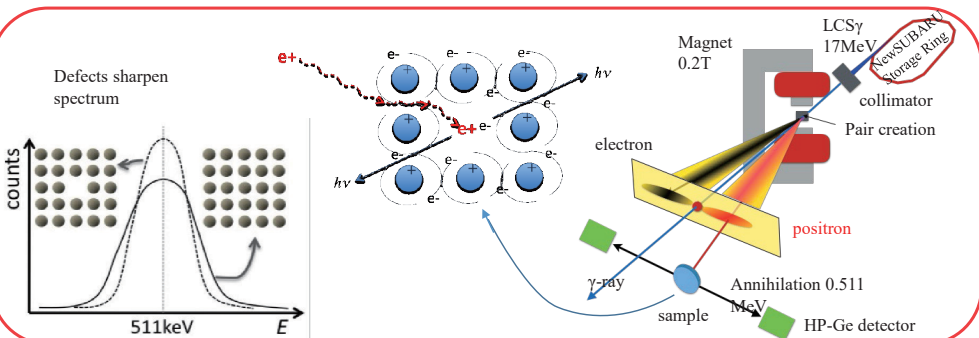


Reference:

- Tsuchiya *et al.*, *Sci. Rep.*, **8**, 3654 (2018)
 Tsuchiya *et al.*, *Biomacromolecules*, **18**, 1002 (2017)
 Tsuchiya *et al.*, *Macromol. Biosci.*, **16**, 1001 (2016)

Inspect nanometer defects in materials

- Used positrons to investigate the number and size of vacancy defects in structural materials and semiconductors
- Enabling the high-precision measurement of material defects using positrons generated from pair-creation by gamma-rays in materials

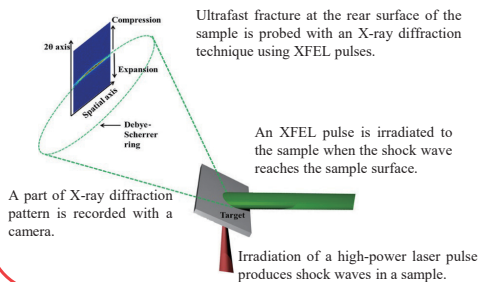


- Reference: Fuminobu Hori, *et al.*, *Positron Science* ("Youdenshi Kagaku" in Japanese), **10**, 21 (2018)

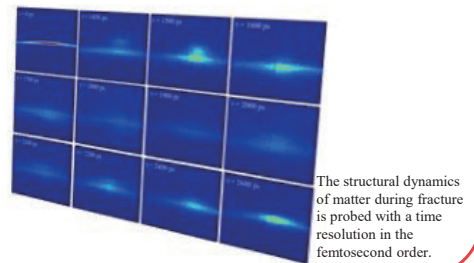
■ Design of material destruction

- Reproduced material destruction in the collision of matter with a speed of 5 km/s by using a high-power optical laser system
 - Studied atomically resolved material fractures with a femtosecond time resolution using an XFEL pulse
- Contributing to the design and development of stronger materials with greater durability

Experimental configuration



Temporal evolution of X-ray diffraction patterns



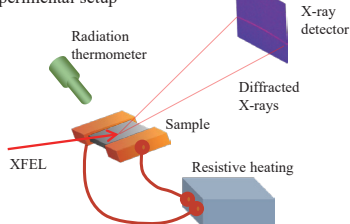
Reference: B. Albertazzi *et al.*, *Sci. Adv.*, **3**, e1602705 (2017)

■ Higher quality and performance for steel

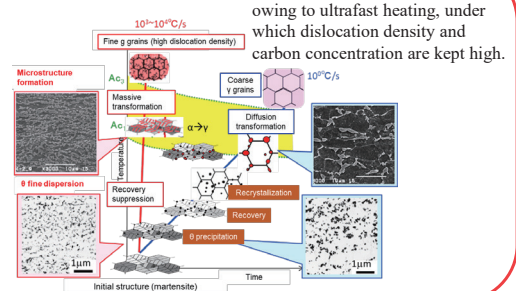
- Observed the structural changes in steel under ultrafast heating *in situ* using time-resolved X-ray diffraction
- Contributing to the production-method development for higher quality steel

Structure changes under heating at a rate of 10000 °C/s were observed using a time-resolved X-ray diffraction technique.

Experimental setup



Process of structural changes

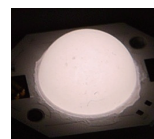
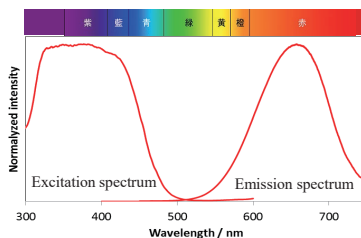
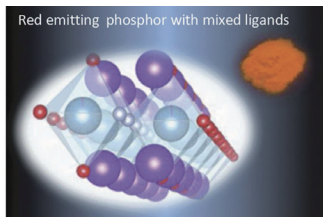


Reference: M. Yonemura *et al.*, *Sci. Rep.*, **9**, 11241 (2019)

Red phosphor for white LEDs

- Development of FOLP: Eu^{2+} , a new phosphor that absorbs light from the ultraviolet to violet spectrum and emits red light
- Elucidation of the luminescence mechanisms of functional materials that enable the control of luminescent color only by their compounding ratio while maintaining high luminous efficiency without absorbing blue to yellow light from structural properties
- Proposing new methods for material search using mixed ligands

FOLP: Structure of the light-emitting site of Eu^{2+}



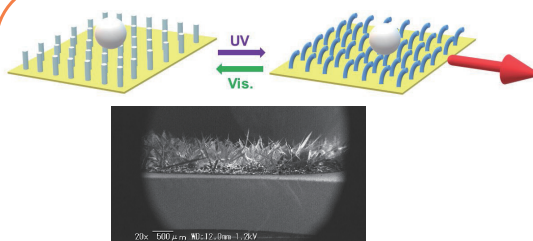
FOLP: Light emission of white LED using Eu^{2+}



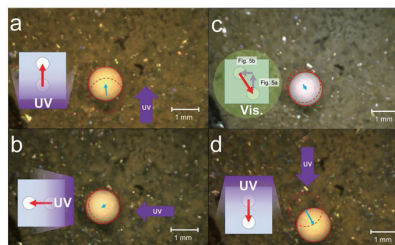
Reference: H. Daicho *et al.*, *Chem. Commun.*, (2017)

Light-controllable object transportation system

- Prepared a photo-actuated smart surface using photo-bendable crystals
- Designed an object transportation system actuated by only light irradiation using a crystalline film
- Developing a crystal brush that can remotely control objects by irradiating possible light



Schematic illustration of the photoactuated smart surface and the SEM image of the crystalline film.



Photographs of transportation of the polystyrene bead upon UV- and visible light irradiation. a) UV-light from the bottom of smart film, b) UV-light from the right side, c) visible-light from the bottom, d) UV-light from the top.

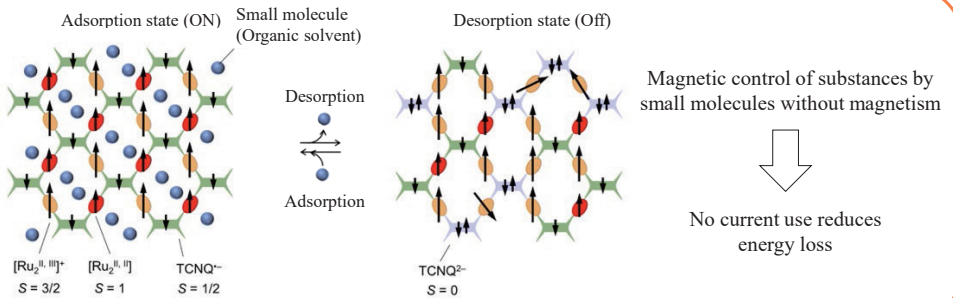
Figures are provided by Ryukoku Univ.



Reference: R. Nishimura *et al.*, *Angew. Chem. Int. Ed.*, **58**, 13308 (2019)

■ Magnetic field control without electric current

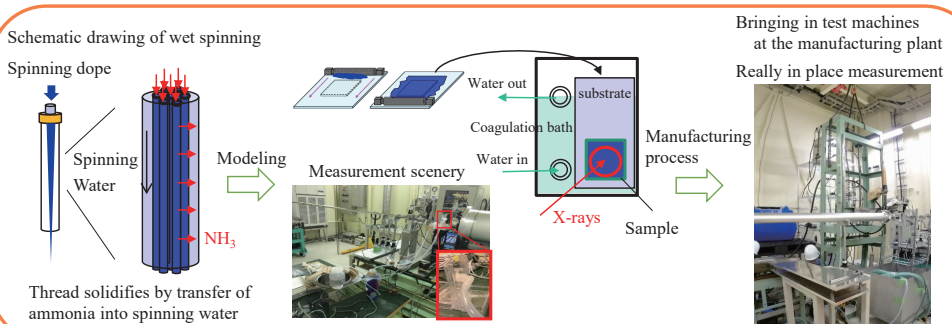
- Designed a material with a structure that changes with the entry and exit of small molecules
 - Proposed a new method to turn on and off the magnetic properties through adsorption and desorption
- Enabling magnetic field modulation without requiring electromagnetic induction



Reference: J. Zhang *et al.*, *J. Am. Chem. Soc.*, **140**, 5644 (2018)

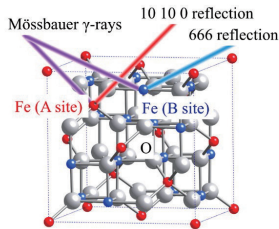
■ Mechanism-based process designing by manufacturing science

- Evaluation of the wet spinning of copper ammonia rayon
 - Measurements taken with a test machine at the manufacturing plant
- Verifying the state of a factory's manufacturing process at a specific point in time

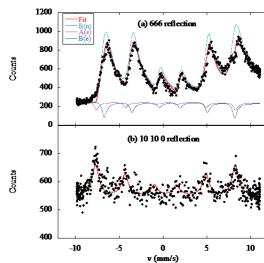


Development guidelines for advanced magnetic devices

- Measuring the crystal site-selective spectra using Mössbauer diffraction
- Obtaining isotope specific information on the electronic and magnetic states, through hyperfine interactions between nuclei and the surrounding electrons
- Contributing to the development of high-performance magnetic and spintronic devices



Conceptual figure of Mössbauer diffraction measurement for $^{57}\text{Fe}_3\text{O}_4$



Mössbauer diffraction spectra of (a) 666 and (b) 10 10 0 reflections

Crystal site selective spectrum measurement was realized as a typical Fe multi-site magnetic compound (magnetite: Fe_3O_4).



The method will be applied to the study of the magnetic and electronic states of various multi-site magnetic materials, which provides guidelines for the development of new magnetic devices.

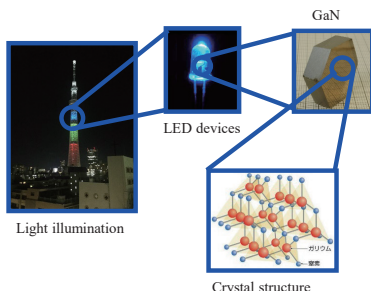


Reference: S. Nakamura *et al.*, *J. Phys. Soc. Jpn.*, **86**, 023706 (2017)

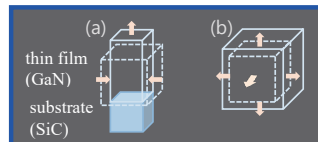
Higher-performance LED devices

- *In situ* X-ray diffraction (XRD) measurements reveal anomalous strain behavior in nitride semiconductor thin films
- Providing vital knowledge to optimize the growth conditions required to produce high-quality LED materials

Gallium nitrides (GaN) in our society



Detailed strain analysis using *in situ* XRD



General thin films are known to be strained elastically (a) to substrates. **GaN thin films** were found to be strained simultaneously both elastically (a) and hydrostatically (b).

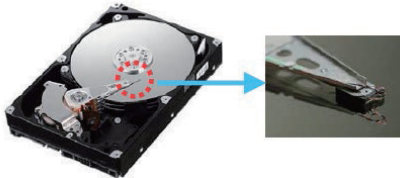
- Vital knowledge to optimize the Ga/N supplying ratio
- Too much gallium-rich ($\text{Ga}/\text{N} \gg 1$) condition leads to low-quality due to the above-mentioned anomalous strain behavior.
- Slightly gallium rich ($\text{Ga}/\text{N} > 1$) is essential to obtain high-quality.



Reference: T. Sasaki *et al.*, *Appl. Phys. Lett.*, **108**, 012102 (2016)

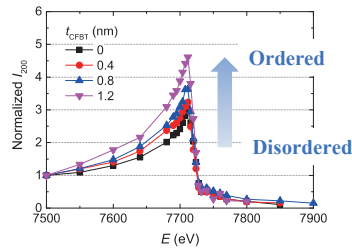
- Data storage for a massively growing data
 - Evaluated structural ordering of Heusler alloys at the atomic level, a candidate for magnetic sensor head materials
 - Improving mass storage for large amounts of information

Disk drive diagram

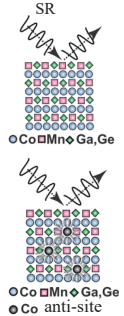


Higher areal density is needed (over 2 Tbit /in²)
→ Atomic order of magnetic sensor head materials is essential

Precise analysis by synchrotron XRD



Evaluating the order with neighboring elements!

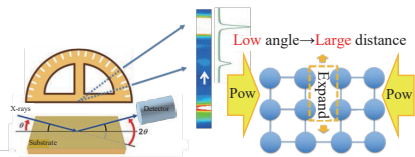
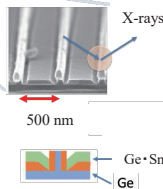


Reference: Li *et al.*, *Appl. Phys. Lett.*, **108**, 122404 (2016); *Acta Mater.*, **142**, 49(2018)
Wang *et al.*, *Acta Mater.*, **166**, 413 (2019)

- Atomic level examinations of electronics materials
 - Evaluated strains precisely in electronics materials using XRD
 - Revealed changes of electric properties by strain, applicable to energy saving
 - Developing new materials with reduced power requirements



Schematic for a smart phone



Strain in electronics materials changes their electronic efficiency

Micro probing by X-ray diffraction (XRD)



Reference: S. Ike *et al.*, *Appl. Phys. Lett.*, **106**, 182104 (2015)

Lead-free piezoelectric materials

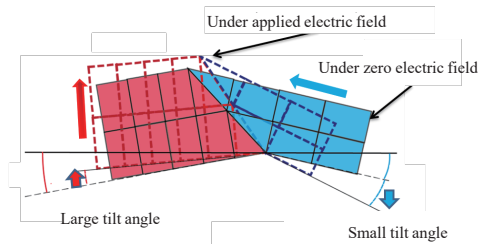
- Observed the ultrafast changes of structures of piezoelectric crystals
- Developing high-frequency ultrafast electromechanical switches and sensors

With electric field

Details of changes in the lattice and the domain structure under applied electric field pulses are still unknown



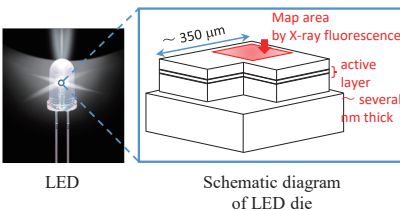
Phenomena that occur simultaneously in the order of nanoseconds was revealed



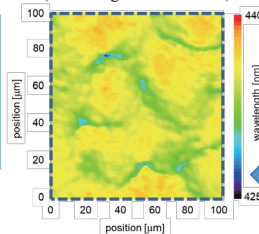
Reference: Y. Eghara *et al.*, *Sci. Rep.* 7, 9641 (2017)

LEDs with higher efficiency

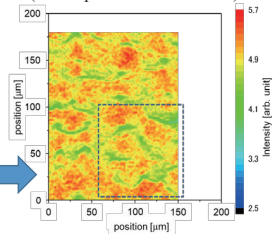
- Visualized the minute composition changes in an active layer of an LED
- Confirmed the correlation between optical characteristics and composition distribution
- Demonstrating the necessity of controlling fluctuations of composition at a nano-micro scale



Optical characteristics
(Wavelength Distribution)



Map by X-ray fluorescence
(Composition Distribution)



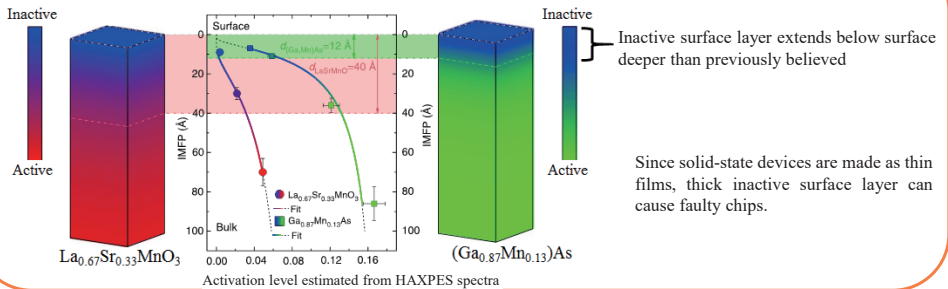
SUNBEAM•Nichia Corporation

Reference: A. Sakaki *et al.*, *Sci. Rep.*, 9, 3733 (2019)

Development of spintronics solid-state devices

- A depth-dependent electronic state was revealed non-destructively for spintronics materials.
 - An inactive surface layer was found to extend deeper than previously believed.
- Determining the critical thickness required to fabricate spintronics devices

Electronic state of spintronics materials investigated by HAXPES

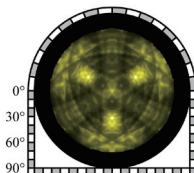


Reference: T. Pincelli *et al.*, *Nat. Commun.*, **8**, 16051 (2017)

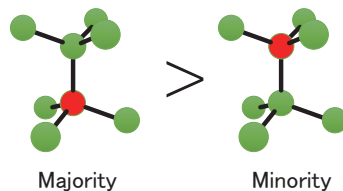
Power devices for efficient energy use

- Observed dopants in diamonds at an atomic scale
 - Revealed a pattern showing where dopants tend to be located
- Developing innovative materials for power devices

Electron wave pattern (photoelectron hologram) of diamond



It was revealed that most of the dopants located at the carbon site and there also was a selectivity of the location.

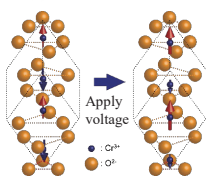


Reference: T. Yokoya *et al.*, *Nano. Lett.*, **19**, 5915 (2019)

Domain wall driven by a magneto-electric effect

- Visualized domain wall creep by transferring weak signals of the anti-ferromagnetic layer to the ferromagnetic layer
- Measured the domain wall speeds
- Creating power-saving, high-speed devices

Appearance of magnetization



Applying voltage creates a difference in the vector size of the up-spin (red arrow) and the down-spin (blue arrow).

Visualization of magnetization of the antiferromagnetic material



When a pulsed electric field is applied under the constant magnetic field, some magnetization reversal region (blue area) appears. We could observe the area gradually spreading.

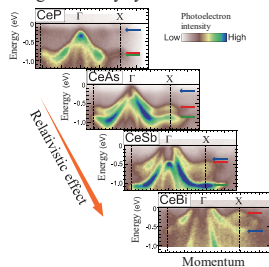


Reference: Y. Shiratsuchi *et al.*, *APL*, **113**, 242404 (2018)
Y. Shiratsuchi *et al.*, *APL Materials*, **6**, 121104 (2018)

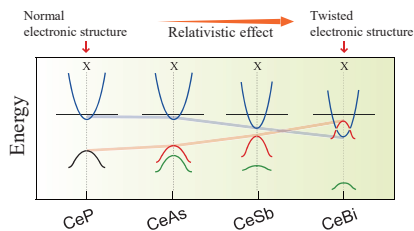
Topological materials for developing ultra-low power consumption devices

- Observed directly the twisted electronic structures corresponding to the topology of materials
- Revealed the mechanisms for forming twisted structures by relativistic effects
- Specifying a new method for determining the topology hidden within a material

Observation of electronic structures using soft X-ray synchrotron radiation



Variation of electronic structures depending on relativistic effect



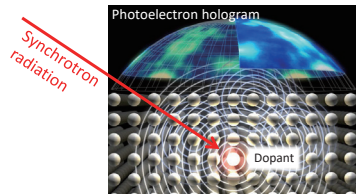
Topology variation in materials can be traced.



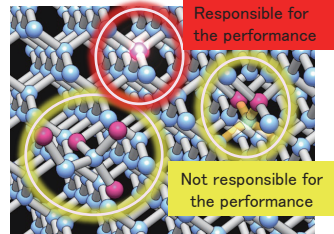
Reference: K. Kuroda *et al.*, *Phys. Rev. Lett.*, **120**, 086402 (2018)

- High performance and low power consumption information devices
 - Atomic-scale observation of dopant locations, determining the performance of semiconductors
 - Developing innovative materials based on local properties

Observation of electron wave pattern from semiconductor silicon



It was revealed that there were several different locations and the location responsible for the performance was determined.

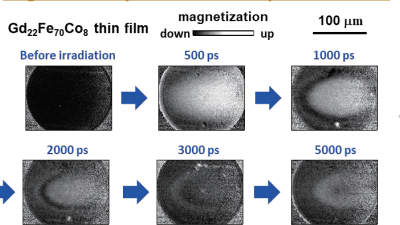


Reference: K. Tsutsui *et al.*, *Nano. Lett.*, **17**, 7533 (2017)

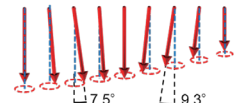
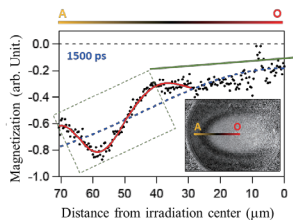
- Power-saving telecommunications technology using magnetization
 - Discovered exceptionally large magnetic waves (spin waves) by applying light pulses to a certain magnetic thin film
 - Controlling magnetic properties in an eco-friendly way by using a non-thermal process of light-induced magnetization

This study aims to realize nonthermal control of magnetic information using “light pulse” instead of conventional methods such as magnetic field, electric pulse, radiofrequency.

Magnetization dynamics after laser pulse irradiation



※ 1ps (picosecond) = 0.000000000001 seconds

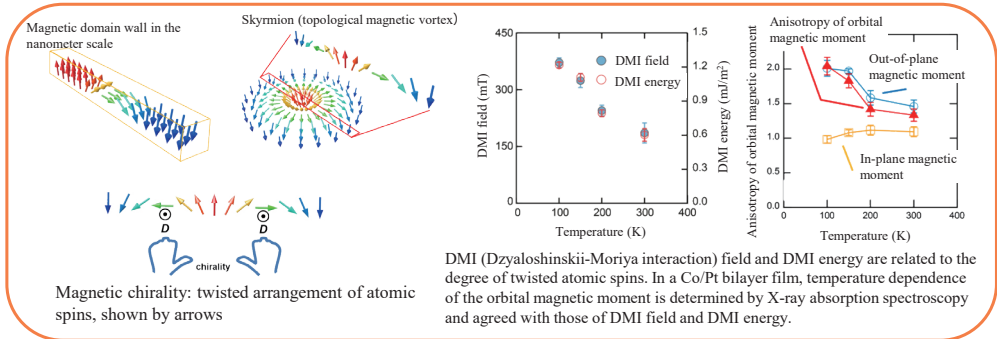


Giant spin waves whose amplitude is about 10 times larger than conventional ones



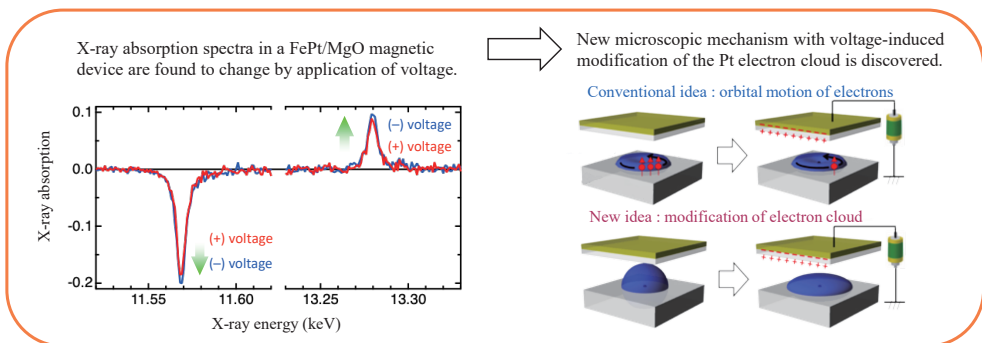
Reference: T. Ohkochi *et al.*, *Appl. Phys. Express*, **10**, 103002 (2017)

- New principle for energy-saving information technology
 - Elucidated the twisted arrangement of atomic spins (magnetic chirality)
 - an important concept for spintronics
 - Creating spintronics devices with extremely high efficiency



Reference: S. Kim *et al.*, *Nat. Commun.*, **9**, 1648 (2018)

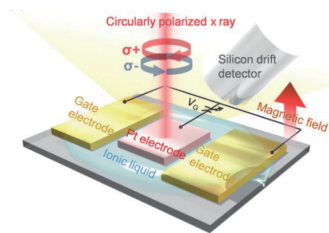
- Magnetic memory devices with ultra low-power consumption
 - Discovered a microscopic mechanism to store digital information that requires extremely low electronic power
 - Developing new magnetic memory devices controlled by deformations at an atomic scale



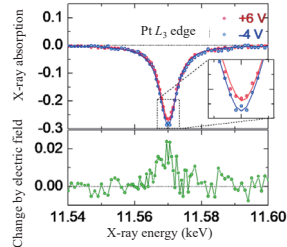
Reference: S. Miwa *et al.*, *Nat. Commun.*, **8**, 15848 (2017)

Controlling magnetic memory with electric fields

- The magnetism and electronic states of a Pt film can be controlled with an electric field.
- Creating microscopic mechanisms for efficient control of magnetic devices



Absorption spectra of circularly polarized X-ray are studied in a Pt/Co device at strong electric fields applied using ionic liquids.



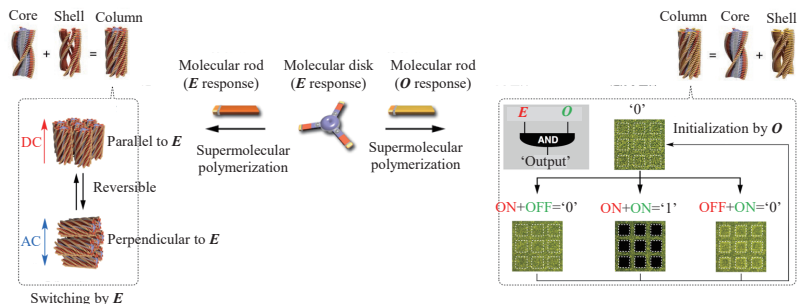
Change in the X-ray absorption spectra of Pt shows the microscopic mechanism of magnetism modified by application of electric field.



Reference: K. T. Yamada *et al.*, *Phys. Rev. Lett.*, **120**, 157203 (2018)

Devices for next-generation optical computing

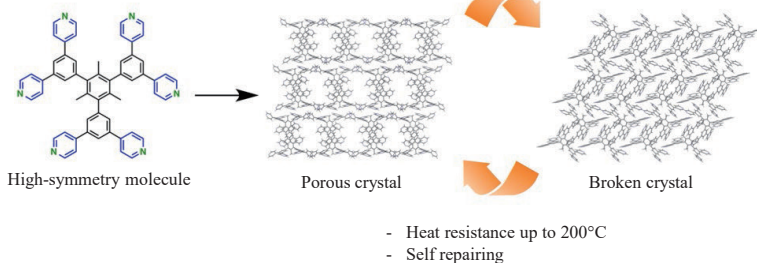
- Development of a functional liquid-crystal using a super-molecular polymerization device operated by electrical (*E*) and optical (*O*) signals
- Developing high-speed, energy-saving devices



Reference: K. Yano *et al.*, *Science*, **363**, 161 (2019)

Maintenance-free materials

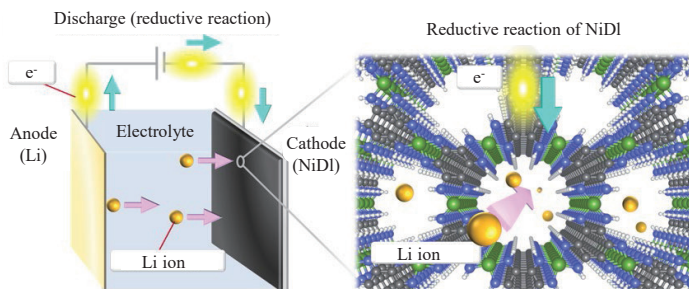
- Development of self-repairable porous crystals with a heat resistance of 202°C
- Realization of damage-free products with crushable zones supported by many reversible bonds



Reference: H. Yamagishi *et al.*, *Science*, **361**, 1242 (2018)

High-performance storage batteries

- Investigating an electronic coordination compound with a flexible crystal structure as a candidate for electrode materials for storage batteries
- Replacing the oxide materials currently used as electrodes

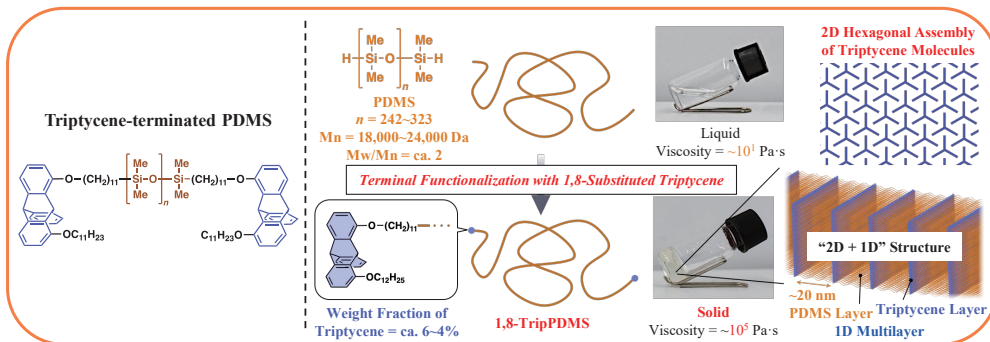


Reference: K. Wada *et al.*, *Angew. Chem. Int. Ed.*, **57**, 8886 (2018)

■ Drastic changes in amorphous polymers

- Developed a new self-assembling motif, different from conventional water-sensitive hydrogen bonding motifs
 - Found an origin for the drastic changes in physical properties of amorphous polymers to be a unique structuring behavior upon terminal functionalization with this motif
- Developing guidelines for designing nano-patterning and transporting materials

former BL45XU

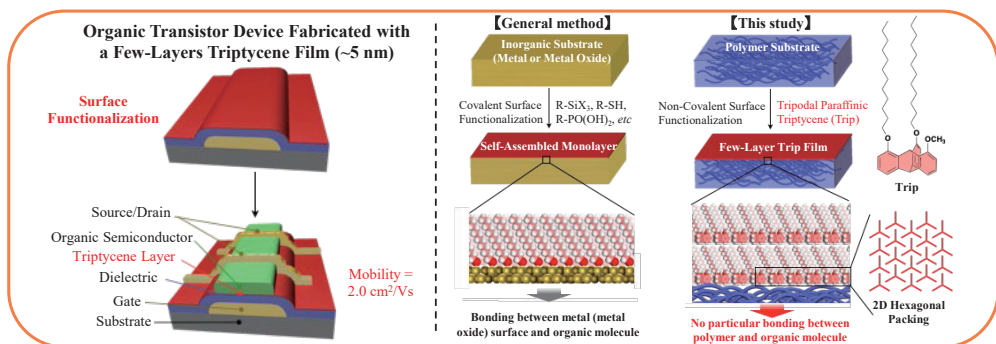


Reference: F. Ishiwari *et al.*, *J. Am. Chem. Soc.*, **140**, 13497 (2018)

■ Higher performance organic transistors

- Fabricated organic thin films with a controlled molecular alignment on various substrates such as plastic and metal and metal oxides
- Developing high-performance flexible organic devices

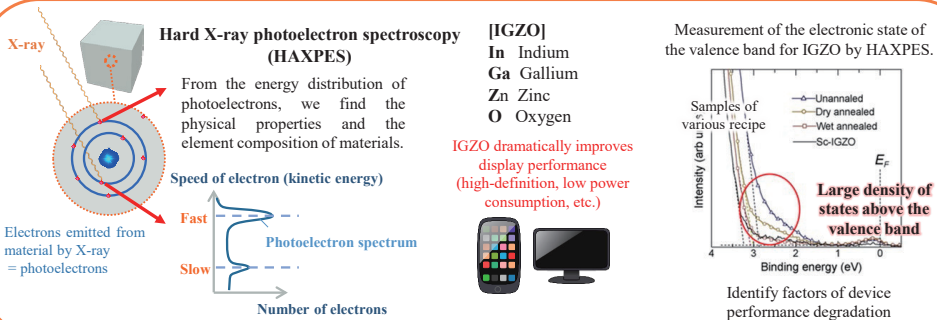
former BL45XU



Reference: T. Yokota *et al.*, *Nat. Nanotech.*, **13**, 139 (2018)

Investigation of physical properties using photoelectrons

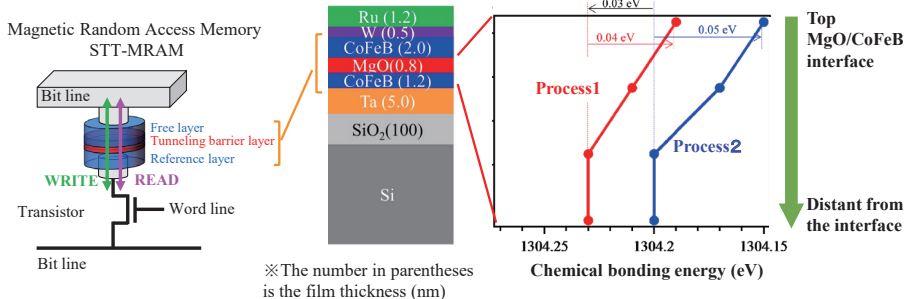
- Using hard X-ray photoelectron spectroscopy (HAXPES) to clarify the composition and electronic states inside solids
 - Determining the causes of performance degradation in oxide semiconductor "IGZO" devices
- Putting high-definition large-screen displays into additional practical uses



Reference: K. Nomura *et al.*, *Appl. Phys. Lett.*, **92**, 202117 (2008)

High-performance memory using spintronics materials

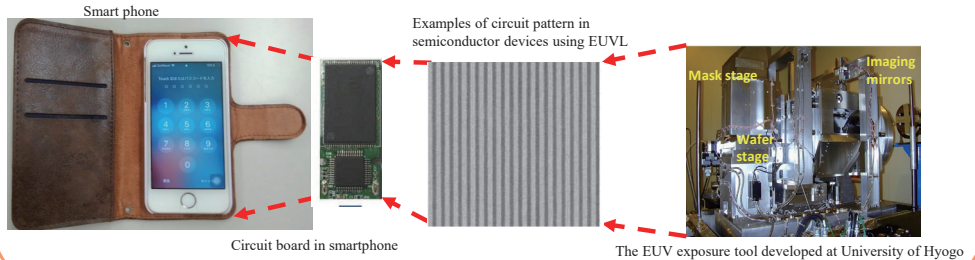
- Established a nondestructive way to examine the physical properties of the MgO tunneling barrier, which determines memory performance
 - Found that the chemical bonding state of the ultra-thin MgO layer depends on the distance from the interface
- Developing next-generation "non-volatile memory" in which the contents are retained even when the power is off



Reference: M. Niwa *et al.*, *J. Appl. Phys.*, **125**, 203903 (2019)

- Fundamental research of extreme ultraviolet lithography (EUVL)
 - Development of optical elements, EUV Mask defect inspections, EUV pellicles, EUV resistant materials, and processing methods
 - Carrying out national projects such as ASET, Selete, EUVA, and EIDEC, and collaborating with international and domestic companies, universities, and research institutes

EUVL technology started to use in high volume manufacturing of 7-nm-node semiconductor devices for the smart phone.

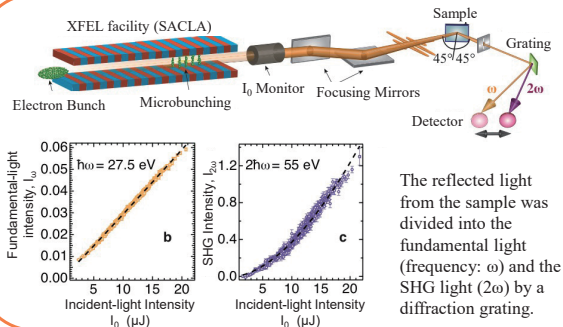


Reference:

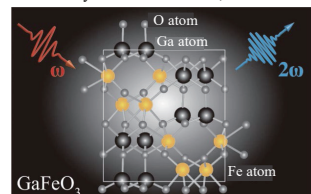
T. Watanabe *et al.*, *Jpn. J. Appl. Phys.*, **36** (12B), 7597 (1997)

T. Watanabe *et al.*, *J. Photopolym. Sci. Technol.*, **29**, 737 (2016)

- Materials mapping with element selectivity
 - Observed the second harmonic generation (SHG) with element selectivity using soft X-ray FEL pulses
 - Demonstrated a technique for probing element distribution and electric properties at interfaces
 - Establishing an element-selective analysis method for nano-device interfaces



The SHG signal from a GaFeO_3 crystal, which has a noncentrosymmetric structure, was observed.



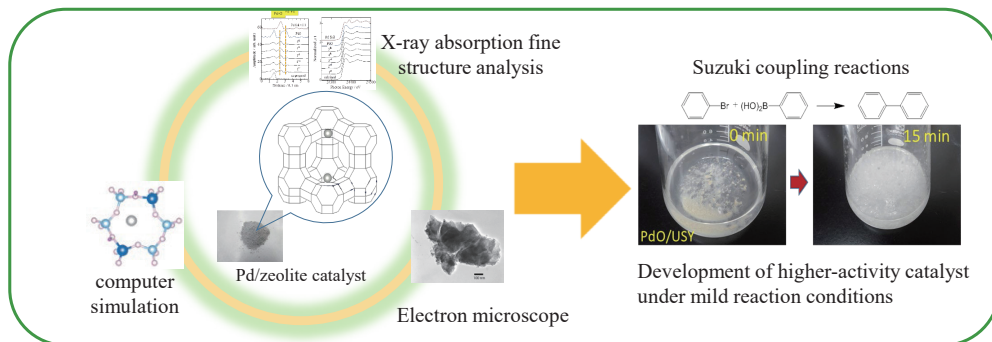
Element selectivity: When the SHG frequency (2ω) matches with the absorption edge of Fe, the SHG signal was enhanced.



Reference: Sh. Yamamoto *et al.*, *Phys. Rev. Lett.*, **120**, 223902 (2018)

High-activity catalysts under mild reaction conditions

- Revealed the structures and chemical states of Pd/zeolite catalysts before and after reactions
- Thermal treatment changes the catalytically active species
- Sharing a new approach for the development of higher-activity catalysts

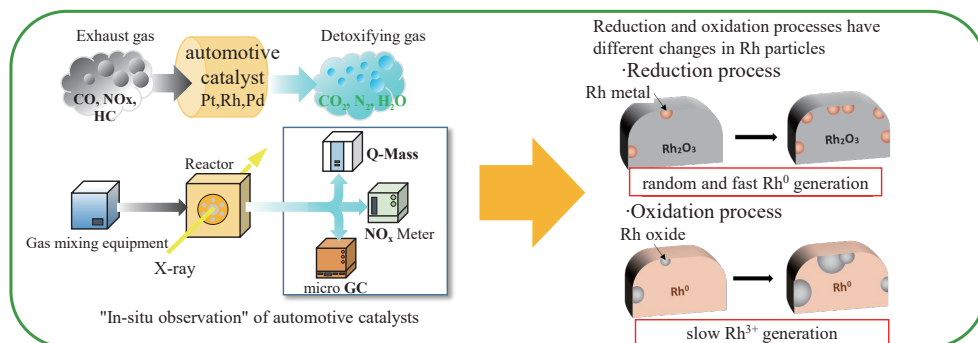


Reference:

K. Okumura *et al.*, *Chem. Phys. Chem.*, **16**(8), 1719 (2015)

Higher-performance automotive catalysts

- Revealed the redox behavior of noble metal components in automotive catalysts using *in situ* observations
- Found differences in the reduction and oxidation processes
- Providing guidelines for reducing the required amount of precious metals and increasing the durability of products

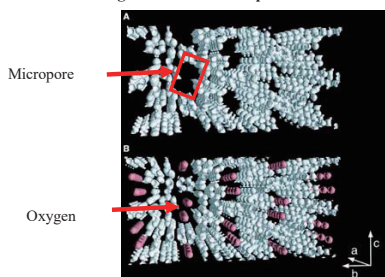


Reference: H. Asakura *et al.*, *J. Am. Chem. Soc.*, **140** (1), 176 (2018)

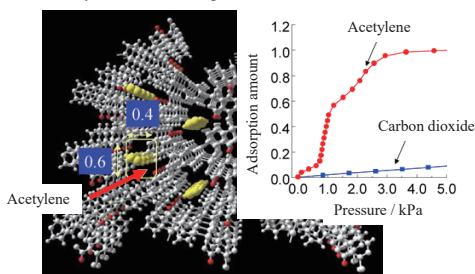
Using hydrogen to reduce global warming

- Observation of regularly arranged oxygen and hydrogen gas in small pores (at a nanometer scale)
- Adsorption of only a specific gas (e.g., acetylene) from a volume of mixed gases
→ Elucidating the mechanisms for selective gas adsorption

Observation of gas inside the micropore for the first time



Acetylene inside micropore



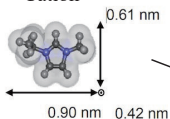
Reference:

- R. Kitaura *et al.*, *Science*, **298**, 2358 (2002)
Y. Kubota *et al.*, *Angew. Chem. Int. Ed.*, **45**, 4932 (2006)
R. Matsuda *et al.*, *Nature*, **436**, 238 (2005)

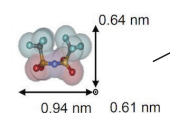
Using a huge current over a short period

- Experimentally verified the theoretical prediction of a “superionic state” in carbon pores
- Found possibility of increasing charge storage by about 100 million times than that of conventional capacitors
→ Developing next-generation electric energy storage devices (super-capacitors)

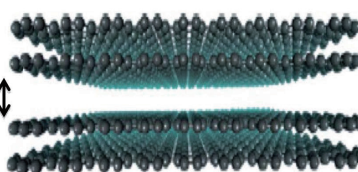
Cation



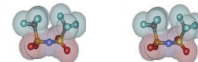
Anion



Slit-shape narrow nanopores (carbon)



Superionic state in the pore



Finding that 25% of the same anion next to the anion

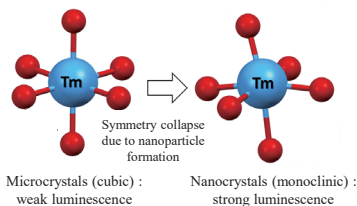
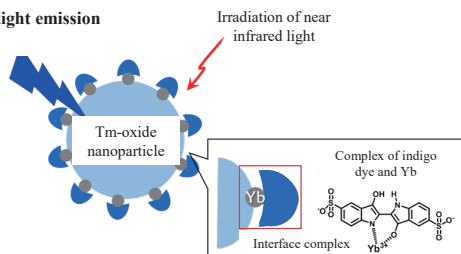
“Superionic state”: a special state that ions of the same charge are gathered and densified in nanopores surrounded by a conductive material



Reference: R. Futamura *et al.*, *Nat. Mater.*, **16**, 1225 (2017)

- Dramatic improvements in solar utilization efficiency
 - Developing nano-particles that convert warm light (near-infrared light) into blue light with high efficiency, and elucidating their structures
 - Improving energy conversion efficiency in conditions of sunlight, artificial photosynthesis, and optical sensors

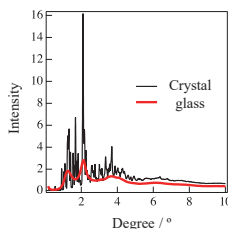
Blue-light emission



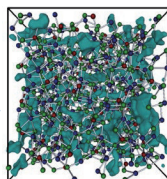
Reference: A. Ishii *et al.*, *Sci. Rep.*, **7**, 41446 (2017)

- Making batteries that are all-solid-state
 - Clarified the structure of a solid (glass) electrolyte to create a solid-state-battery
 - Elucidated a mechanism for providing performance higher than that of conventional batteries
 - Developing commercial products by combining experiments and theory

Development of new solid electrolytes for next-generation batteries through understanding of glass structures



High energy X-ray
total scattering
+
Simulation



Understanding glass structures that satisfies both experiment and theory



Development of
battery materials
used in automobiles
and airplanes

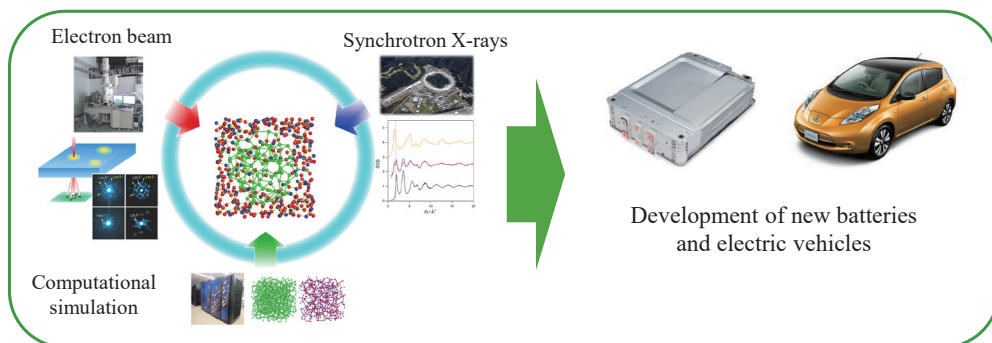
Images are provided by Toyota



Reference: K. Ohara *et al.*, *Sci. Rep.*, **6**, 21302 (2016)

■ Understanding the mechanisms of batteries

- Observation of the atomic arrangement of the electrodes in a battery that contained non-uniform and disordered structures
 - Visualization of non-uniform structures in battery material for the first time
- Accelerating battery development by combining electron beams, synchrotron X-rays, and theoretical calculations



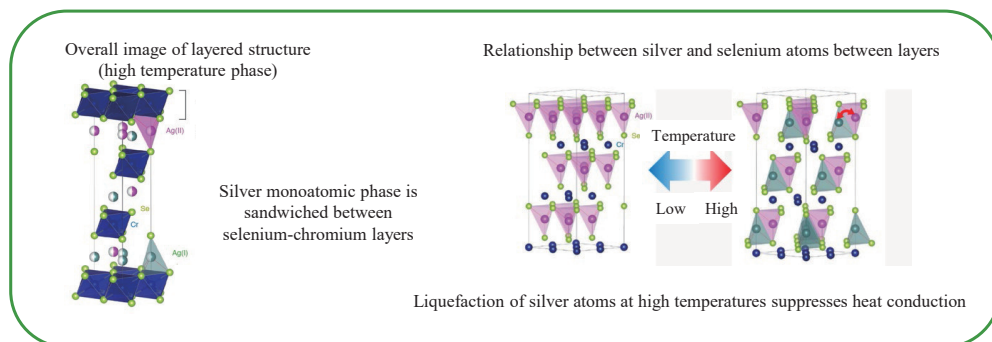
Images are provided by Nissan



Reference: A. Hirata *et al.*, *Nat. Commun.*, **8**, 15549 (2017)

■ Highly efficient thermoelectric materials

- Clarification of the mechanisms by which silver chromium selenide efficiently converts heat into electricity
- Understanding more clearly the behavior of liquids, leading to improved performance for thermoelectric materials

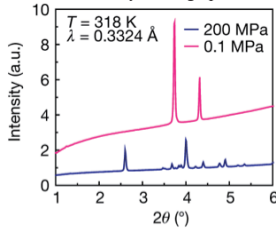


Reference: B. Li *et al.*, *Nat. Mater.*, **17**, 226 (2018)

New cooling technology using solid refrigerants

- Elucidation of the mechanisms that cause "plastic crystals" to exhibit ten times larger heat generation and endothermic capabilities than those of conventional solid refrigerants
- Providing an approach for next-generation cooling technologies

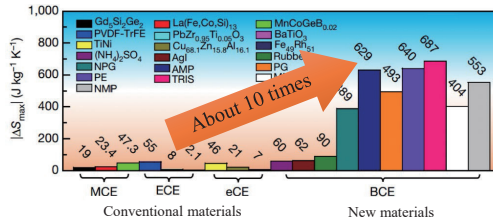
X-ray diffraction of plastic crystals at ordinary and high pressure



Crystal structure changes from face-centered cubic lattice to monoclinic system by applying pressure



Entropy change of calorimetric materials



This structural transition can greatly reduce entropy



Reference: B. Li et al., *Nature*, **567**, 506 (2019)

Lithium-ion battery development using machine learning and mathematics

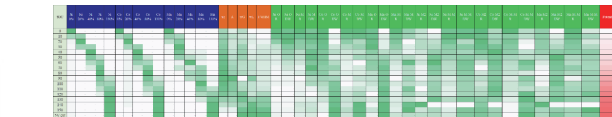
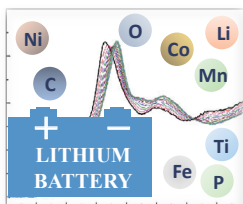
- Using SR analyses and machine learning in combination with advanced data analysis will be highly effective for developing superior battery materials
- Improving performance for the batteries used in hybrid cars, electric vehicles, and home appliances

Synchrotron X-ray studies during the charging and discharging of Lithium-ion batteries are carried out to collect big data.

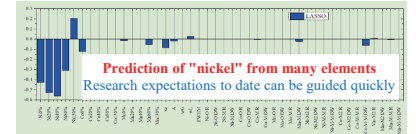
Many kinds of batteries consisting of various elements and their content ratio are used as test samples.

Machine Learning and data analyses have been executed to reveal the key element for performance of batteries.

Components of lithium-ion batteries are made up of various elements.



Prediction of elements which greatly affect battery performance



Prediction of "nickel" from many elements
Research expectations to date can be guided quickly

Effective element prediction from mass data in a short period of time

Speeding-up of R&D

Realization of high-performance lithium-ion battery

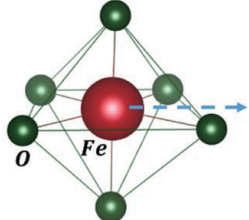


These results are based on joint research with KOBE STEEL, Ltd. and KOBELCO research institute, Inc.

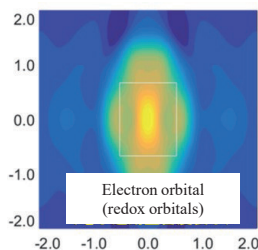
New techniques for diagnosing batteries

- Successful visualization of electron orbitals (redox orbitals), which are important factors that determine the performance of lithium-ion batteries
- Improving the diagnosis and performance of lithium ion battery by direct observation of electron orbits

Positive electrode material: FeO_6 octahedral structure of olivine-type lithium iron phosphate



Redox orbit of iron (Fe) in the center of octahedron



Redox orbital changes and battery
The change in potential is proportional



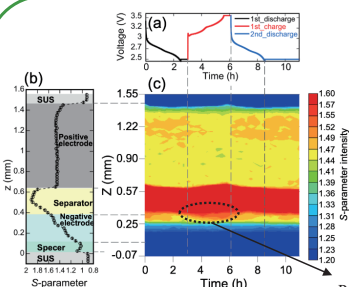
Quantitative evaluation of battery potential shift



Reference: H. Hafiz *et al.*, *Science Advances*, **3**, e1700971 (2017)

In situ observation of the operating state of batteries

- Clarification of changes in the lithium composition of positive and negative electrodes during battery charge and discharge cycles
- Eliminating causes of battery deterioration and contributing to the development of higher performance batteries



(a) Charge / discharge curve of a battery. The process in which the battery voltage reaches 3.5V to 2.5V is the discharging process, and the process in which the battery voltage reaches 2.5V to 3.5V is charging.

(b) From the S-parameters obtained from Compton scattering measurements, the internal structure of the battery can be determined.

(c) Change in lithium ion concentration distribution during charge / discharge process

Discovered that lithium ions have accumulated between the separator and the negative electrode during charging



Elucidation of the factors affecting commercial battery deterioration

Precipitation of lithium species



Reference: K. Suzuki *et al.*, *J. Synchrotron Radiat.*, **24**, 1006 (2017)

Examining the interiors of large batteries

- Development of a non-destructive method for observing the inside of a large lithium-ion battery in operation
- Developing higher performance and safer storage batteries, including for automobiles

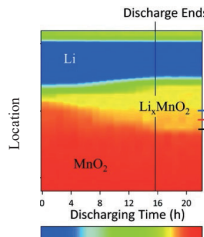
Irradiates high energy X-rays and measures scattered X-rays from inside the commercial battery



Conventional battery cell for X-ray measurement: thinner cell so that X-rays can be transmitted



Real product :
Normal X-rays cannot penetrate



Developing a method that can measure the battery of commercial products as it is



Direct observation of how lithium on the negative electrode decreases with discharge and enters the positive electrode

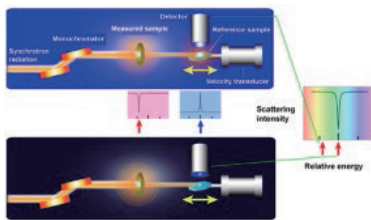


Reference: M. Itou et al., *J. Synchrotron Radiat.*, **22**, 161 (2015)

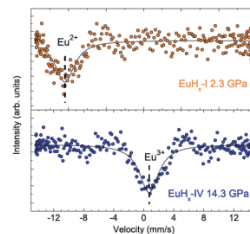
Understanding how hydrogen is stored in materials

- Elucidating the properties of hydrogen storage materials to make progress toward a "hydrogen society"
- Controlling the reactivity, crystal structures, and hydrogen concentration

Very tiny samples under the ultra high pressure can be measured.



Principle of synchrotron radiation
Mössbauer spectroscopy



Divalent state under the low pressure



Trivalent state under the high pressure

Mössbauer spectra for Europium hydride

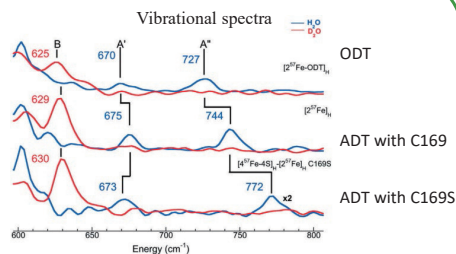
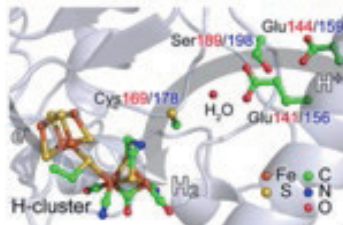


Reference: Matsuoka et al., *Phys. Rev. Lett.*, **107**, 025501 (2011)
Seto et al., *Phys. Rev. Lett.*, **102**, 217602 (2009)

Information for the design of artificial enzymes

- Resolved the positions of hydrogen atoms in hydrogenase
 - Discovered that activity is affected by the surrounding environments not directly bonded to the hydrogen atoms
- Creating high efficiency enzymes to enable an eco-friendly hydrogen society

Hydrogen flow near the active center in hydrogenase



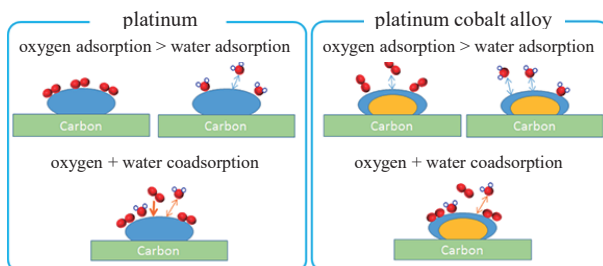
Vibration of hydrogen atoms is affected by the surrounding environment.



Reference: Reijerse *et al.*, *J. Am. Chem. Soc.*, **139**, 4306 (2017)

Moving toward a “hydrogen society”

- Revealed wetting-induced oxidation in platinum-based catalysts for fuel cells using *in situ* observation
 - Identified degradation mechanisms of catalytic efficiency under humidified atmosphere
- Developing guidelines for improving catalysts



In platinum, oxygen and water enhance the oxidation cooperatively and the coadsorption deteriorates the performance of fuel cell.



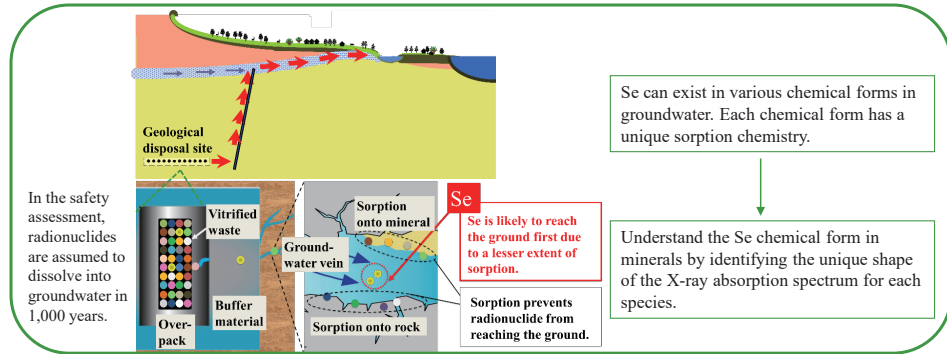
In platinum cobalt alloy, the wetting induced oxidation was found to be suppressed.



Reference: Y. Cui *et al.*, *Sci. Rep.*, **7**, 1482 (2017)

Developing a “mineral” for the safe disposal of geological materials

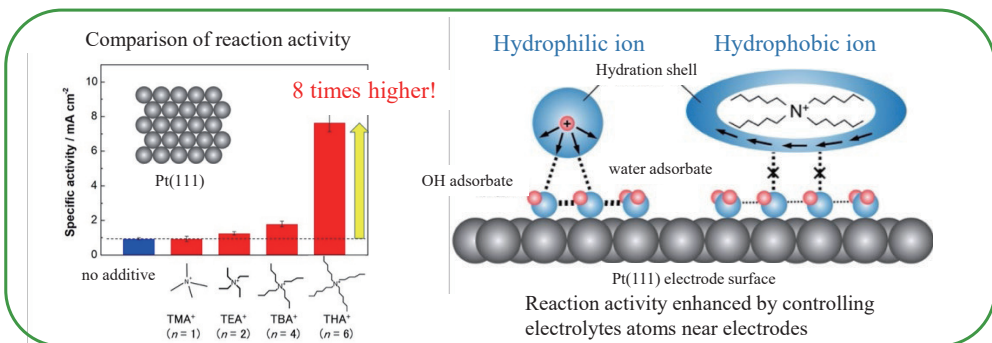
- Clarified the causes of the retardation of radionuclide migration by sorption onto minerals and rocks after dissolving into groundwater in the repository environment
- Elucidating the sorption mechanisms of Se on minerals



Reference: R. Doi *et al.*, *J. Nuc. Sci. Technol*, **53** (10), 1554 (2016)

More efficient power generation

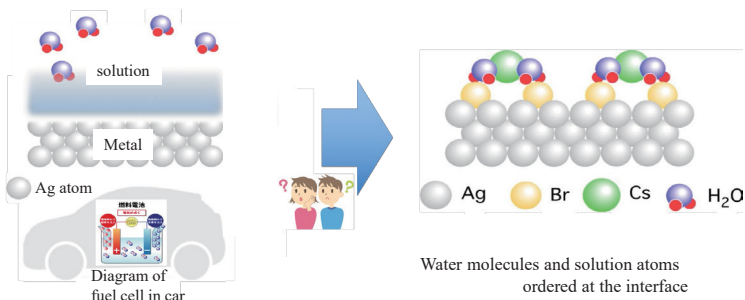
- Revealed atomic arrangements at the solid-liquid interface using X-ray diffraction (CTR scattering)
- Achieving activation of fuel cell reactions that are eight times higher by using a small amount of additives



Reference: Kumeda *et al.*, *Nat. Commun.*, **9**, 4378 (2018)

- A key to investigate the interfaces in fuel cells
 - Observed the ordering of water molecule and solution atoms
 - Utilized CTR (crystal truncation rod) scattering sensitive to surface/interface
- Observing unique atomic behavior at the interface

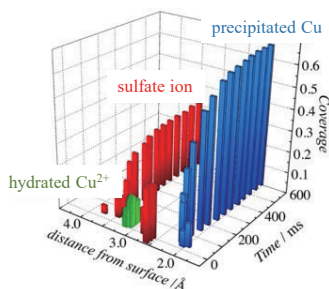
How do atoms behave at the metal/solution interface?



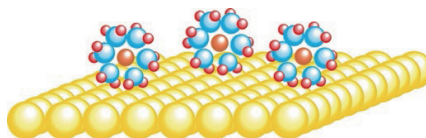
Reference: Nakamura *et al.*, *J. Phys. Chem. C*, **118**, 22136 (2014)

- Highly active catalysts
 - Succeeded in real-time observation of interfacial ions during electro-crystallization
 - Found the concentration of counter anions to be the factor that determines the deposition rate
- Fabricating nano-particle catalysts by controlling the deposition rate of ions

Time evolution of structural parameters



Hydrated metal ions before precipitation

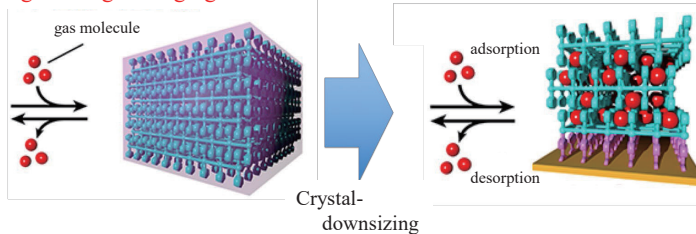


Reference: Nakamura *et al.*, *Sci. Rep.*, **7**, 914 (2017)

Thin film storing gas

- Evaluated lattice constants of coordination framework thin films
- Observed a dynamic guest-sorption behavior in thin films
- Developing functional materials for switching or sensor devices

Diagram of gas straging film



The gate is closed in the bulk.

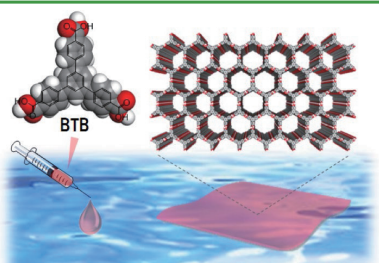
Thin film storages gas by gate-opening.



Reference: Sakaida *et al.*, *Nat. Chem.*, **8**, 377 (2016)

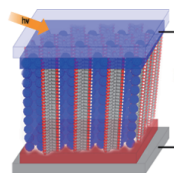
Nanosheets: innovative solar cell materials

- Fabricated nano-sheets on water surfaces
- Fabricating 3D nano-building for inorganic solar cells or separation membranes at ambient conditions



BTB solution is dropped on water surface.

BTB forms nanosheet with nanopores.



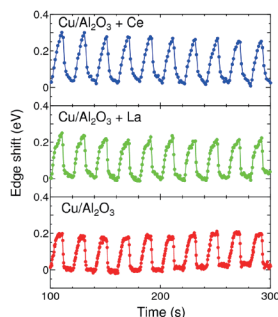
Construction of the ordered structure two kind of molecules are arranged alternately, which is ideal for inorganic solar cell.



Reference: Makiura *et al.*, *ACS Nano*, **11**, 10875 (2017)

- Exhaust gas purification that does not require precious metals
 - Developing catalysts without precious metals
 - Improving the functionality of catalysts by using copper with additional elements
 - Developing higher performance catalysts

XAFS measurements during exhaust gas purification



Ce addition



La addition



Without addition



Purification performance

High

Low

Additives to Cu improve catalytic performance



Reference: Y. Nishihata, D. Matsumura, *Journal of JSSRR*, **26**, 57 (2013)

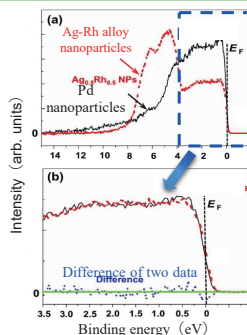
- Storage hydrogen like noble metals
 - Investigated the immiscible bulk for Ag and Rh (which are unable to form alloys)
 - Found the hydrogen storage capabilities of Ag-Rh alloy nano-particles, achieved under specific conditions with their arrangements about 10 to 20 nanometers in size
 - Achieving similar behavior of electrons in Ag-Rh alloys as seen in Pd metal

Three successive metallic elements in the periodic table

45 Rhodium(Rh)	46 Paradium (Pd)	47 Silver (Ag)
		
Cannot storage	Can storage	Cannot storage

Very small nanoparticles are miscible and store hydrogen !

Investigate reason by synchrotron X-rays



Electronic structure of Ag-Rh alloy is similar to that of Pd metal

Reason for the capability of absorbing/storage hydrogen

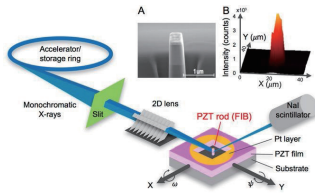


Reference: A. Yang et. al., *Appl. Phys. Lett.* **105**, 13109 (2014)

Higher efficiency power generated material by vibration

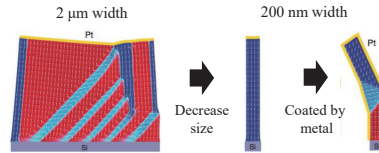
- Observed the atomic arrangement of a nanorod of $\text{Pb}(\text{Zr}_{0.35}\text{Ti}_{0.65})\text{O}_3$
- Discovered the behavior of domain structures modified by the size of a nanorod and its environment
- Improving energy transfer capabilities by controlling domain structures

Synchrotron X-ray diffraction measurement of a nanorod



X-ray beam was focused onto a single PZT rod.

Difference in the size of nanorod and its environment



Domain structure, which determines the energy transfer capability, can be modified by the size of nanorod and its environment.

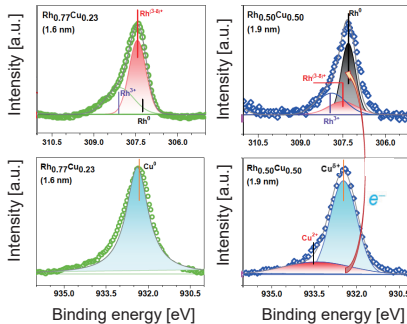


Reference: T. Yamada *et. al.*, *Sci. Rep.* 7, 5236 (2017)

Development of innovative catalysts

- Observation of electronic states of several Rh-Cu alloy nanoparticles
- Discovering similar catalytic activities for Rh-Cu alloy nanoparticles at different Rh-to-Cu ratios

High-resolution HAXPES data



Nanoparticles are covered with polyvinylpyrrolidone (PVP) to prevent them from clumping together. For Rh-Cu NPs with Rh-rich composition, Rh atoms existing in the surface layer of nanoparticles turn to Nano $\text{Rh}^{(3-\delta)+}$ as they release an electron to the PVP.



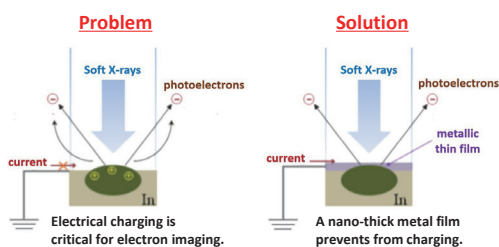
Rh-Cu NPs with comparable Rh:Cu ratio, electrons move from Cu to Rh, resulting in the formation of Cu^{2+} , decreased $\text{Rh}^{(3-\delta)+}$ and increase Rh^0



Reference: N. Palina *et. al.*, *Sci. Rep.* 7, 41264 (2017)

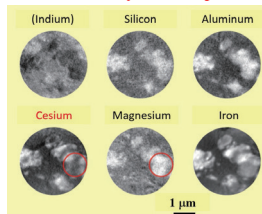
Cleaning up contaminated land in Fukushima

- Used photoemission electron microscopy to investigate clay mineral particles that can artificially absorb cesium atoms
- Providing a new method for elucidating cesium adsorption mechanisms



Element-specific nano-spectroscopic analysis of clay particles is now possible.

Elemental distribution map of Cs-adsorbed clay mineral particles



Inverse distribution is recognized between cesium and magnesium, indicating that preferred cesium adsorption site is strongly influenced by local valence states in the particle.

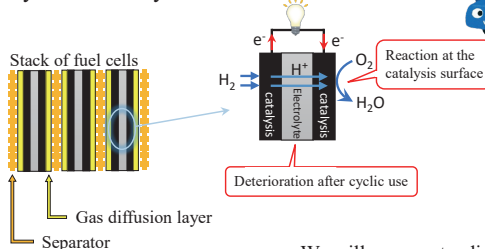


Reference: A. Yoshigoe *et al.*, *Appl. Phys. Lett.*, **112**, 021603 (2018)

Long-life and high-quality fuel cells for the future

- Observed chemical reactions at the catalysis surface in polymer electrolyte fuel cells
- Elucidating the reaction and deterioration mechanisms in fuel cells

Polymer Electrolyte Fuel Cell



Towards clean and ecological car

Soft X-ray absorption / emission spectroscopy

⇒ Observation of change in the chemical state of oxygen molecules

Soft X-ray spectromicroscopy

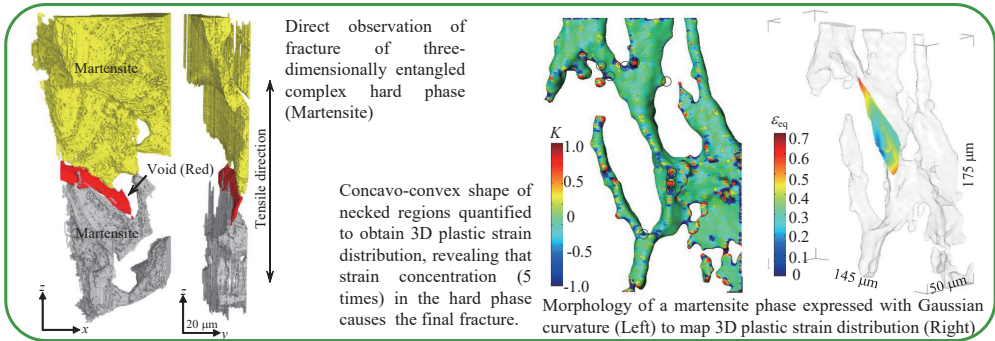
⇒ Observation of distributions of water molecule and metallic ions in the membrane of electrolyte

We will carry out a direct observation of working fuel cell in near future.



Reducing CO₂ emissions by decreasing automobile body weight

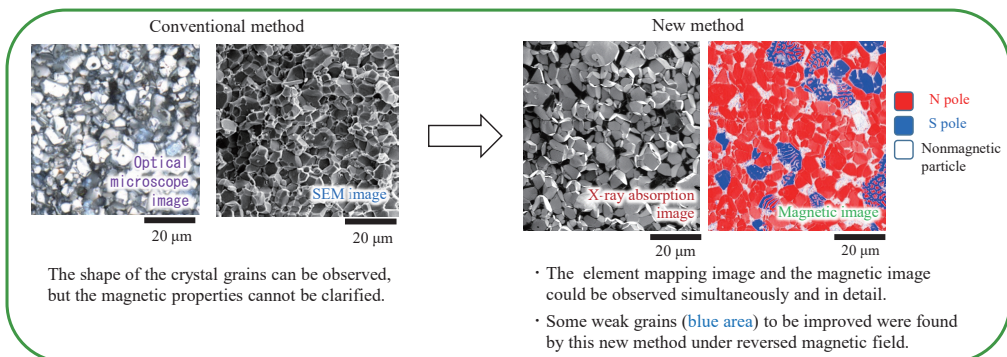
- Used a phase contrast imaging technique to visualize dual phase structures in high-performance DP steels by utilizing subtle density differences
- Revealed fracture mechanisms by visualizing fracture behaviors in 4D (i.e., time evolution in 3D)
- Achieving higher performance in automotive steel sheets



Reference: H. Toda *et al.*, *Acta Materialia*, **126**, 401 (2017)

More eco-friendly cars and higher efficiency wind-power generators

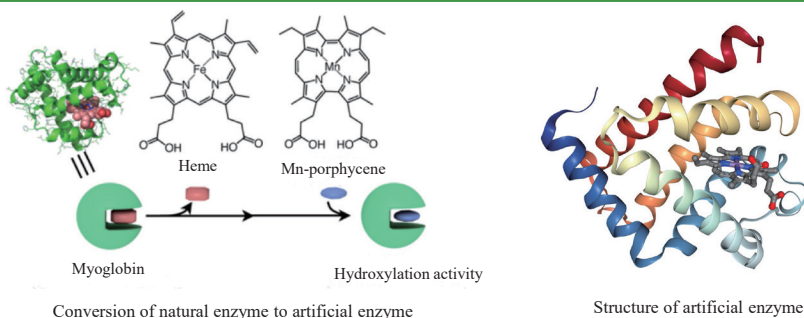
- Development of a microscope for clearly observing magnetic domains under high magnetic fields
- Developing permanent magnets that have no rare elements and provide higher performance



Reference: Y. Kotani *et al.*, *J. Synchrotron Rad.*, **25**, 1444 (2018)

Catalytic mechanisms of artificial enzymes

- Incorporation of a metal complex (Mn-porphycene) into heme-binding proteins can generate a reactive intermediate for the catalytic hydroxylation of C–H bonds.
 - X-ray analysis revealed the 3D structure of the metal active sites in artificial enzymes.
- Designing a perfect catalyst that can transform natural hydrocarbons into useful products

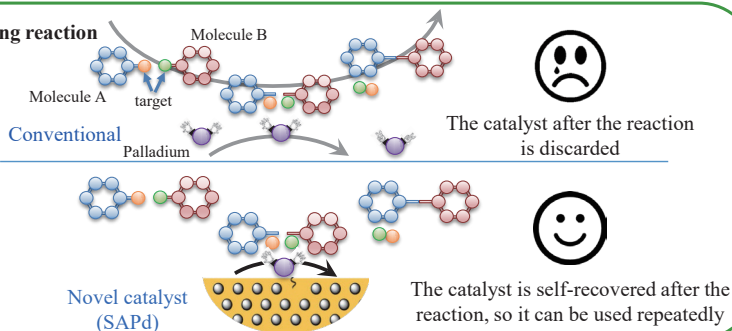


Reference: K. Oohora *et al.*, *J. Am. Chem. Soc.*, **139**, 51 (2017)

Development of a sustainable catalyst

- Clarified the structure of a new catalyst that can be used repeatedly
- Developing a safe catalyst with low leakage and contributing to significant reductions in precious metal usage in chemical synthesis

Palladium cross-coupling reaction



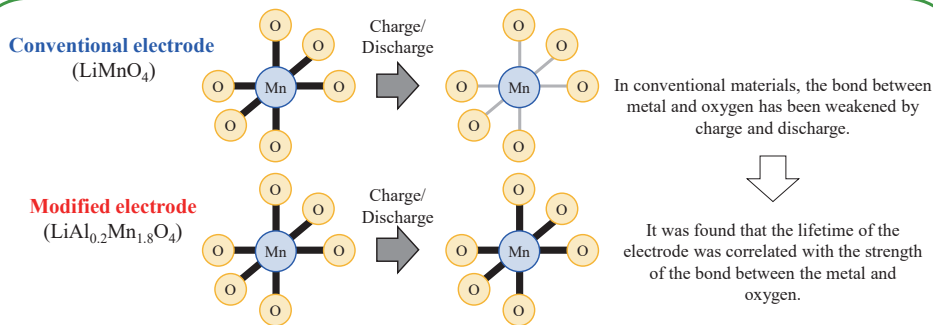
Reference:

M. Arisawa *et al.*, *RSC Advances*, **5**, 676 (2015)

T. Akiyama *et al.*, *ACS Appl. Nano Mater.*, **1**, 12, 6950 (2018)

More durable lithium-ion batteries

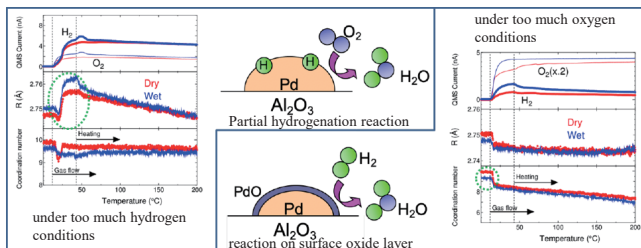
- Elucidation of the importance of maintaining the bonds between transition metal and oxygen to slow the deterioration of lithium-ion batteries
- Developing new battery materials with a greater lifespan to sustain repeated charging and discharging



Reference: D. Asakura *et al.*, *Phys. Chem. Chem. Phys.*, **19**, 16507 (2017)

Storage of hazardous waste

- Analyzed the reaction mechanisms of “honeycomb-type hydrogen safety catalysts”
- Confirmed that hydrogen safety catalysts can reduce the hydrogen concentration in a storage container below the lower explosive limit
- Developing safer and longer lasting storage for hazardous waste from the Fukushima Nuclear Power Plant



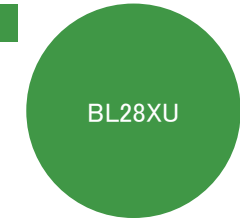
The material having noble metal surface that can be easily reduced shows catalytic activity even in a humid atmosphere.



Reference: Matsumura *et al.*, *Int. J. Hydrog.*, **42**, 7749, (2017)

BL28B2

- Developing higher performance fuel cells

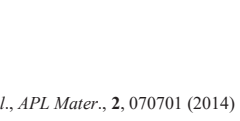


Reference: Imai *et al.*, *J. Am. Chem. Soc.*, **131**, 17 (2009)

BL28XU

BL28XU

- Elucidating reaction mechanisms during high-speed charge-discharge processes

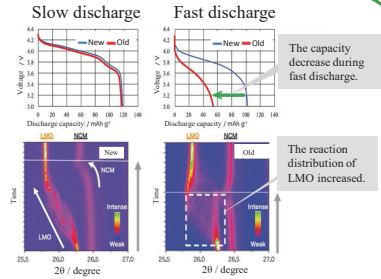
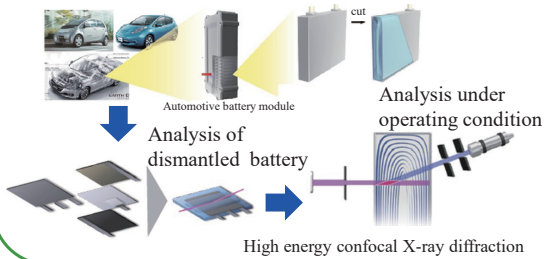


Reference: K. Tokuda *et al.*, *APL Mater.*, **2**, 070701 (2014)

Improving the performance of storage batteries

- Developed a high-energy confocal X-ray diffraction method to evaluate battery degradation mechanisms
- Detected the characteristic differences between new and old batteries during slow and fast battery operation
- Clarifying the causes of degradation for storage batteries and improving battery performance

Analysis of products recovered from the market



The cause of battery degradation was revealed.



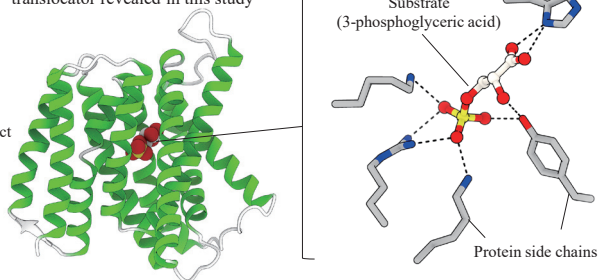
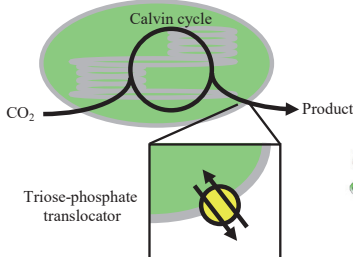
Reference: H. Fujimoto *et al.*, *IJAE*, **45**, 297 (2014)

Basis for plant gene modification and artificial photosynthesis

- The triose-phosphate translocator is an exporter of photosynthetic products from the chloroplasts.
- The crystal structures revealed the counter-exchange mechanisms for three substrates.
- Answering a 40-year-old question regarding how photosynthesis works

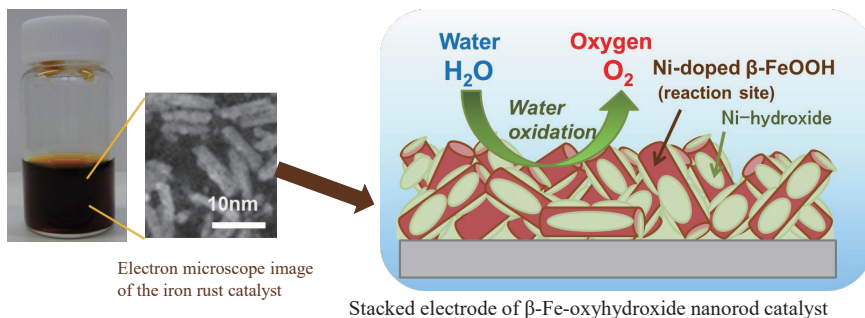
Discovery of photosynthetic product exporters from chloroplasts in 1960s–70s

Structure of triose-phosphate translocator revealed in this study



Reference: Lee *et al.*, *Nature Plants*, **3**, 825-832 (2017)

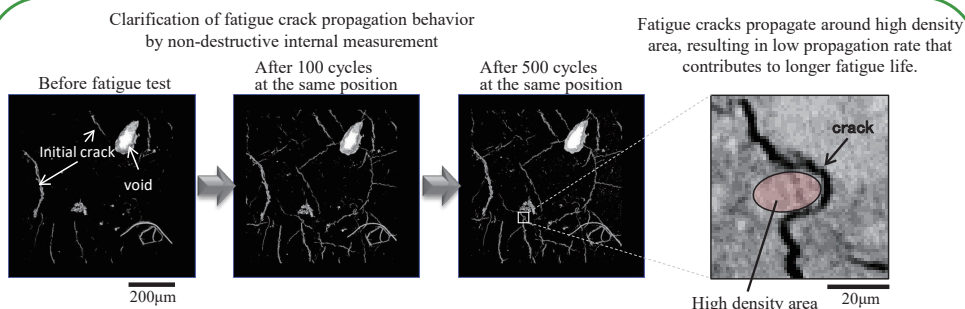
- Producing organic compounds from CO_2 and H_2O using sunlight energy
 - Elucidation of the atomistic structures of highly active iron rust catalysts, β -Fe-oxyhydroxide nanorod, for a water oxidation reaction to produce oxygen
 - Developing a system composed of earth-abundant elements that enables artificial photosynthesis



Reference:

T. M. Suzuki, T. Morikawa, *et al.*, *Bull. Chem. Soc. Jpn.*, **91**, 778 (2018)

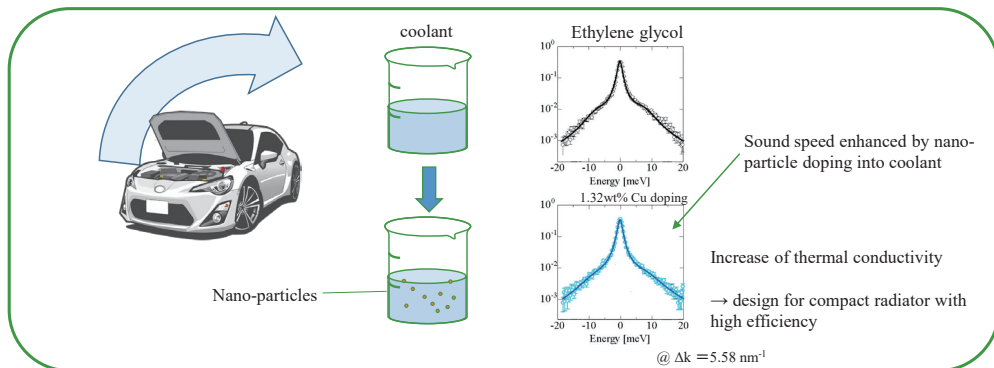
- Improving the eco-friendliness of electric vehicles
 - Clarified the internal fatigue crack propagation behavior in the bonding layers of power modules in a nondestructive manner
 - Improving the reliability of core components of vehicle electrification and reducing environmental impacts



Reference:

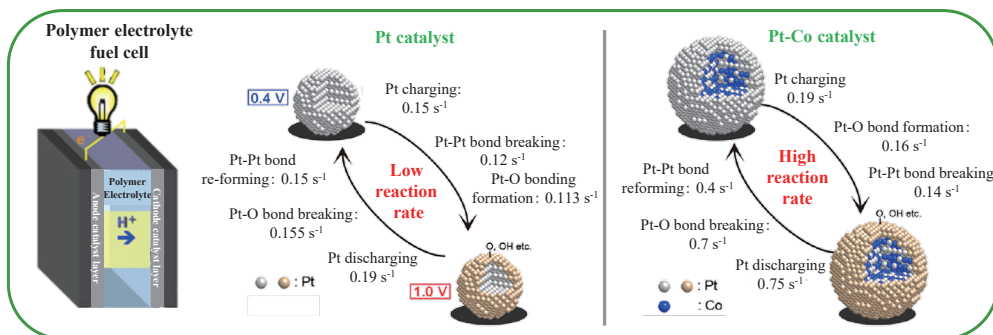
M. Usui, H. Kimura, *et al.*, *Microelectronics Reliability*, **63**, 152 (2016)

- Design for more compact automobile parts to reduce energy consumption
 - Investigating atomic-scale thermal conductivity of nano-particle-doped coolants with high thermal conductivity
 - Using coolants with a higher heat exchange rate and developing more compact drive trains for automobiles



Reference: K. Yano *et al.*, *J. Molecular Liq.* **248**, 468 (2017)

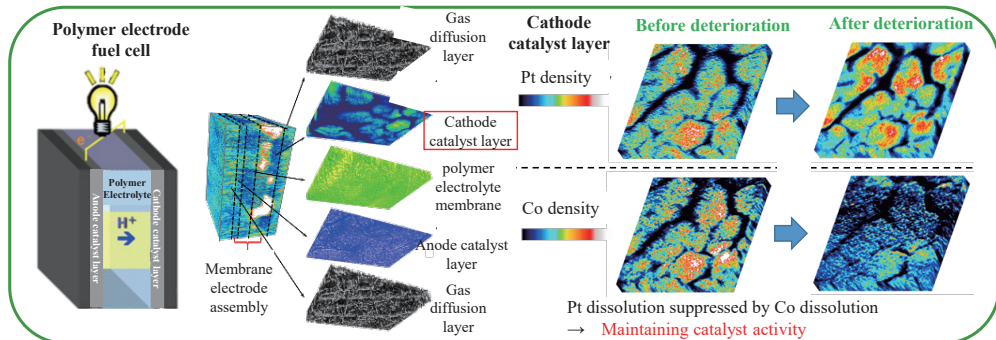
- Clarifying catalytic reaction mechanisms of polymer electrolyte fuel cells
 - Used time-resolved XAFS to measure the rate constants of the elementary steps of electrode catalytic reactions
 - Constructed a redox reaction model of Pt and Pt-Co catalysts
 - Improving the durability of Pt-Co catalysts and achieving superior performance for fuel cells



Reference: N. Ishiguro *et al.*, *J. Phys. Chem. C*, **118**, 15874 (2014)

High durability fuel cell electrodes

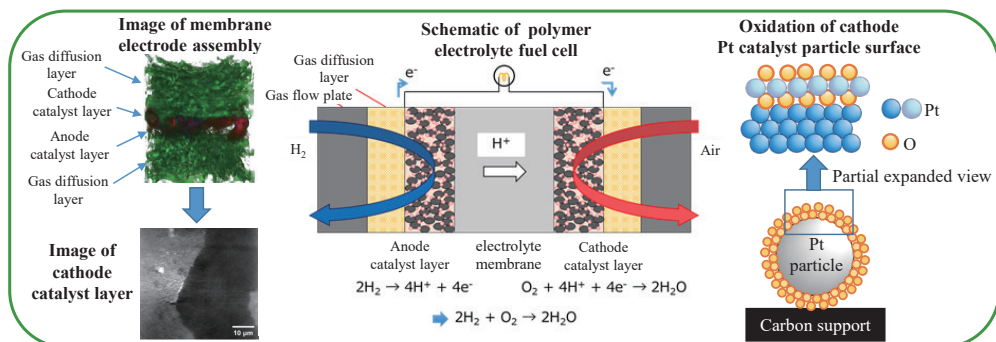
- Visualized the 3D chemical states of electrode catalysts under polymer electrolyte fuel-cell operating conditions
 - Clarified the deterioration mechanisms of fuel cell by measuring the chemical states and structures of electrode catalyst layers
- Clarifying the high durability mechanisms of Pt-Co catalysts



Reference: Y. Tan *et al.*, *J. Phys. Chem. C*, **123**, 18844 (2019)

Next-generation fuel cell electrode catalysts

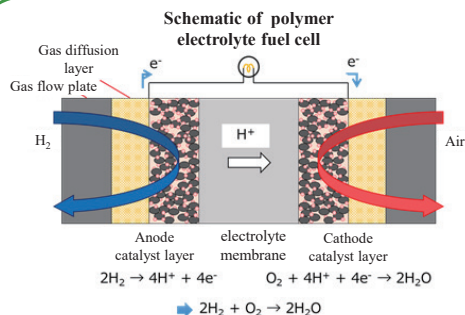
- Developed a simultaneous/sequential multi-analysis system
 - Completed an operando analysis for complex fuel cells
- Providing information for the design of new fuel cell electrode catalysts



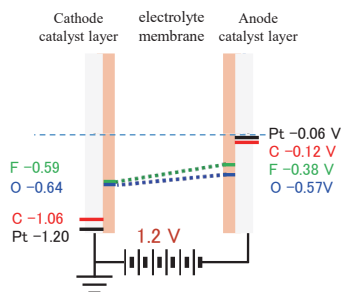
Reference: T. Uruga *et al.*, *Chem. Rec.*, **19**, 1444 (2019)

Electrochemical phenomena in fuel cells under operating conditions

- Measured for the first time the X-ray photoelectron spectra under real ambient pressure
- Succeeded in measuring the voltage in fuel cells and of the poisoning of electrode catalyst particles
- Developing innovative powerful tools for analyzing fuel cells and catalyst materials



Measurement of voltage in fuel cell without tester

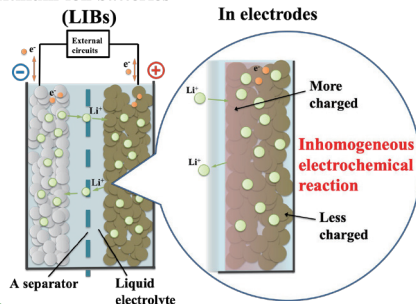


Reference: Y. Takagi, *et al.*, *Appl. Phys. Exp.*, **10**, 076603 (2017)
L. Yu, *et al.*, *Phys. Chem. Chem. Phys.*, **19**, 30798 (2017)

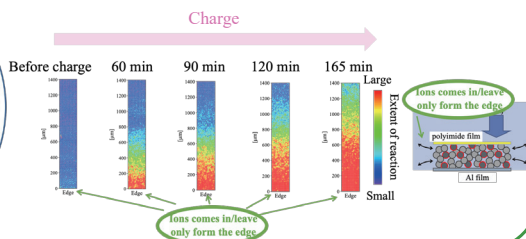
High-performance lithium-ion batteries (LIBs)

- Visualized the electrochemical reactions in LIBs during battery operation
- Finding new insights for designing high-performance LIBs

Lithium-ion batteries (LIBs)



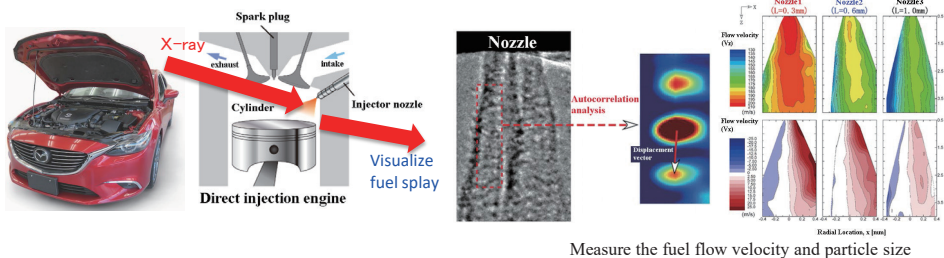
Inhomogeneous reaction evolution was successfully visualized



Reference: T. Nakamura *et al.*, *J. Phys. Chem. C*, **121**(4), 2118 (2017)
T. Nakamura *et al.*, *Batteries Supercaps*, **2**, 688 (2019)

- Developing fuel-efficient engines for eco-friendly vehicles
 - Analyzed the relationship between the structures of injection nozzles and fuel spray using single- and multi-exposure X-ray imaging
 - Analyzing the spray structures and dynamics to design more fuel-efficient injection nozzles for automobiles

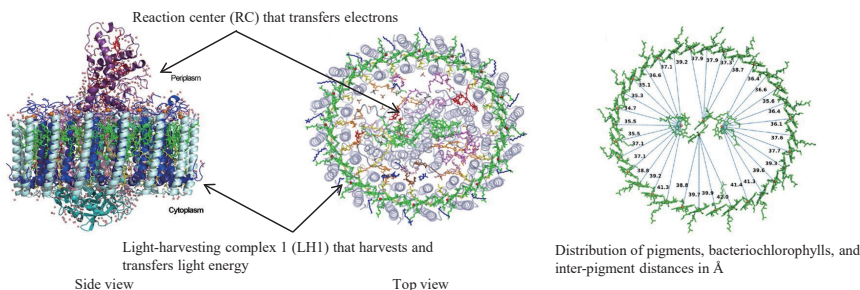
Analyze the structure and dynamics of fuel spray using X-ray imaging



Reference:

S. Moon *et al.*, *Exp. Therm. Fluid Sci.*, **68**, 68 (2015)

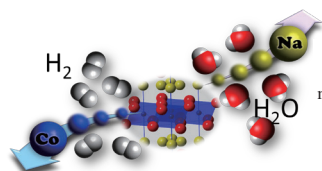
- Improvements in solar energy
 - Determined the structure of the photosynthetic LH1-RC supercomplex in photosynthetic bacteria
 - Revealed the mechanisms for light energy absorption, transfer, and conversion into chemical energy with high efficiency
 - Developing guidelines for using solar energy with high efficiency



Reference: L. J. Yu *et al.*, *Nature*, **556**, 209 (2018)

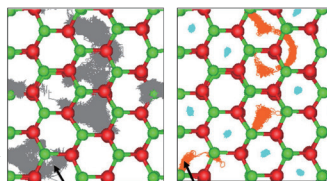
- Effective use of hydrogen as a clean energy source
 - Simulations based on the observations of hydrogen motion in a solid-state battery
 - Developing solid-state batteries powered by water and hydrogen

Power generation from H_2O and H_2 in an oxide



Exchange of Na for H_2 and O_2

Simulation of moving hydrogen



Hydrogen path

Oxygen path

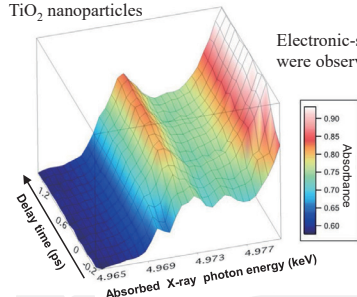
New battery materials



Reference: K. Kato *et al.*, *Chem. Asian J.*, **11**, 1537 (2016)

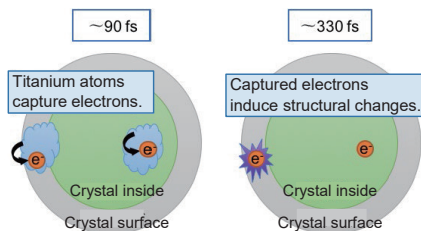
- Electron motion in photocatalysts
 - Observed the electronic-state changes in photo-excited TiO_2 nanoparticles using time-resolved X-ray absorption spectroscopy with 100-fs temporal resolution
 - Contributing to the development of high-performance catalysts through a better understanding of the mechanisms of catalytic reactions

Time-resolved X-ray absorption spectra of photo-excited TiO_2 nanoparticles



Electronic-state changes were observed.

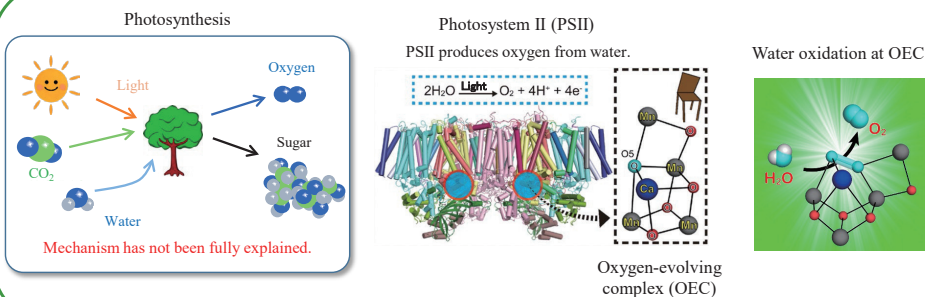
Model of time development after the photo-excitation.



Reference: Y. Obara *et al.*, *Struct. Dynam.*, **4**, 044033 (2017)

Revealing the secrets of photosynthesis

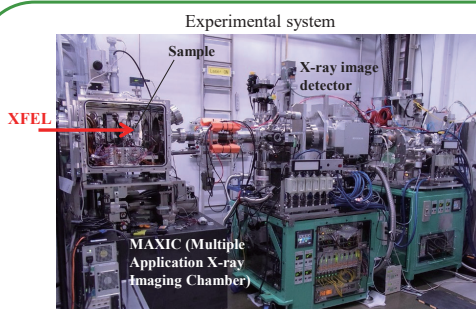
- Determined the structure of photosystem II, a catalyst in the water-splitting and oxygen-evolving reaction
 - Measured the structure of the reaction intermediate in which an oxygen molecule is formed at the center of the reaction
- Understanding the mechanisms that drive photosynthesis



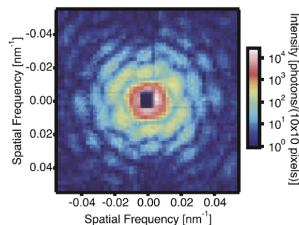
Reference: M. Suga *et al.*, *Nature*, **517**, 99 (2015)
M. Suga *et al.*, *Nature*, **543**, 131 (2017)
M. Suga *et al.*, *Science*, **366**, 334 (2019)

Damage-free analysis of catalysts

- Nano-scale observations of catalysts for cleaning automotive exhaust gas without radiation damage
 - Development of observation methods applicable to various materials in solutions
- Contributing to operando analysis of catalysts under actual use conditions



Coherent diffraction pattern of a three-way catalyst sample



Analysis for image reconstruction gave an image of an alumina carrier holding rhodium nanoparticles.

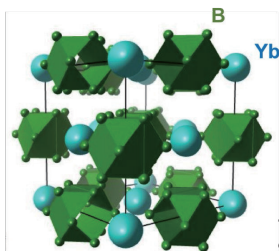


Reference: R. Yoshida *et al.*, *J. Phys. B* **48**, 244008 (2015)

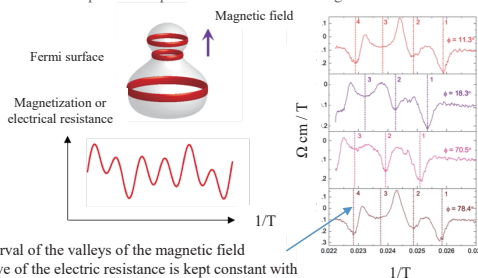
Discovering new physical phenomena in insulators

- Observation of quantum oscillations in which the electrical resistance and magnetic susceptibility of an insulator change based on a magnetic field
- Determination of the crystal structure and the purity of an insulator exhibiting quantum oscillation
- Developing new theoretical proposals and experiments

Crystal structure of YbB_{12} showing quantum oscillation



Relationship between quantum oscillations and magnetic field



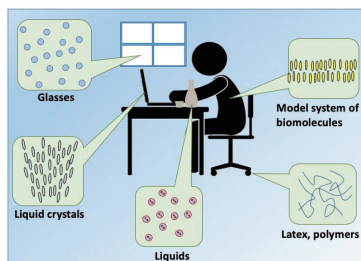
The interval of the valleys of the magnetic field derivative of the electric resistance is kept constant with respect to the reciprocal of the magnetic field



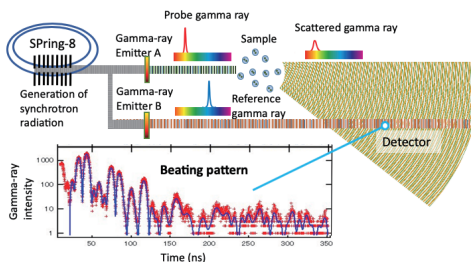
Reference: Z. Xiang *et al.*, *Science*, **362**, 65 (2018)

Observing the atomic and molecular dynamics at a rate of 1/10,000,000 sec

- Development of precise measurement methods with ten times higher efficiency
- Analyzing practical materials such as liquid crystals, rubbers, and new electrolytes



Properties of the familiar materials can be studied in detail by the atomic and molecular dynamics

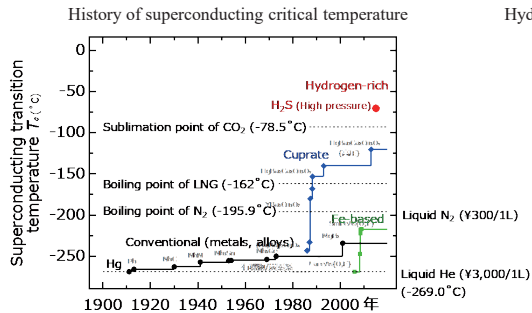


More than 10 times higher efficiency has been realized by the multi-line method

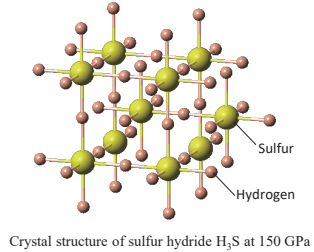


Reference: Saito *et al.*, *Sci. Rep.*, **7**, 12558 (2017)

- Achieving the long-held dream of “superconductivity at room temperature”
 - Determined the crystal structure of highly compressed hydrogen sulfide during the surprisingly high-temperature superconducting phase at -70°C
 - Providing new clues for the quest to develop next-generation high-temperature superconductors



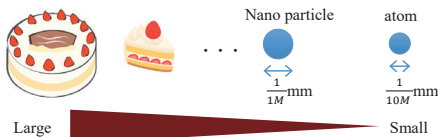
Hydrogen-rich compounds become superconducting at high pressure.



Reference: M. Einaga *et al.*, *Nat. Phys.*, **12**, 835 (2016)

- New nano-particle science
 - Studying nano-particles with standard X-ray techniques (XRD, EXAFS, *etc.*)
 - Investigating the size effect of nano particles
 - Discovering new exotic physical properties of nano particles

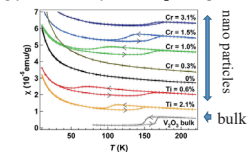
Size effect of physical properties



- Increase area of surface → chemical reaction
- Few impurities → uniformity of sample
- Surface property dominates physical properties than normal bulk property
- Interest for Solid State Physics

Nano particle experiment

Strongly correlated system VO_2 nano particles



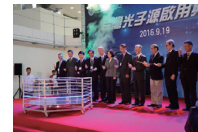
Magnetic susceptibility

Physical properties change with particle size



Reference: Y. Ishiwata *et al.*, *Adv. Mater. Interfaces*, **2**, 1500132 (2015)
J. Jiao *et al.*, *Nat. Chem.*, **11**, 222 (2019)

- Taiwan Photon Source (TPS) – a third-generation 3.0 GeV synchrotron light source
 - Location: Hsinchu Science Park in Hsinchu, Taiwan
 - The Taiwan Light Source (TLS) is a second-generation 1.5 GeV synchrotron radiation facility that also operates at this site
 - Providing a third-generation 3.0 GeV synchrotron source that offers high brilliance and low emittance



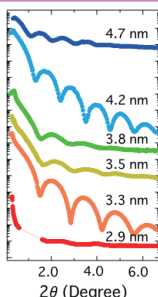
TPS opening ceremony

- 23 beamlines are operation at TLS(2019)
- 17 beamlines(Phase-II) will be in operation by end of 2020
- Another 9 beamlines(Phase-III) will be prepared by 2025

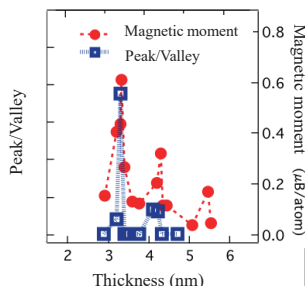


Reference: Homepage of NSRR : <https://www.nsrrc.org.tw/>

- Adjusting magnetic states through structural electronic engineering
 - Investigated the close relations among distortion, quantum-well states, and magnetization
 - Found a stabilization mechanism for ferromagnetism in Pd ultra-thin films
 - Investigating the possibility of magnetic-switching with distortion



X-ray reflectivity



Thickness vs magnetic moment

In-situ fabrication of ultra-thin film in ultra-high vacuum

Pd ultra-thin film shows spontaneous distortion via the appearance of ferromagnetism!

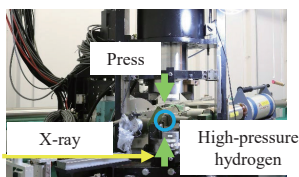
Ferromagnetic Pd results in flatter and uniform film growth!



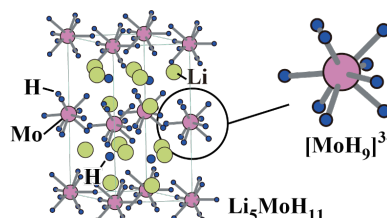
Reference: Sakuragi *et al.*, *Phys. Rev. B* **97**, 21421 (2018)

Synthesis of innovative hydrides

- Identified high hydrogen coordination to synthesize innovative hydrides
 - Synthesized innovative transition metal hydrides complexes with nine-fold hydrogen coordination
- Developing applications for high performance batteries



High-pressure hydrogenation technique have been developed using in-situ synchrotron radiation x-ray diffraction measurements.



X-ray and neutron diffraction measurements and theoretical calculation confirmed the formation of ninefold hydrogen coordination

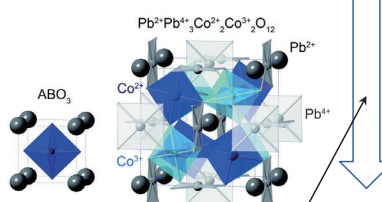


Reference: S. Takagi *et al.*, *Sci. Rep.*, 7, 44253 (2017)

Fabrication of lead perovskites and the discovery of charge ordering

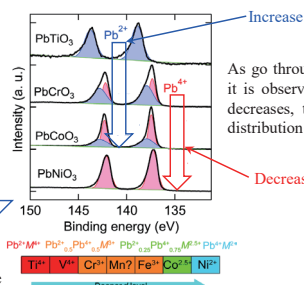
- Fabricated lead cobaltate
 - Discovered unusual charge ordering in both Co and Pb
- Developing innovative oxide materials based on the controlling valences of elements

Crystal structure determined by synchrotron X-ray diffraction measurements



Left to right in the periodic table

Observation of behavior of electrons by synchrotron X-rays



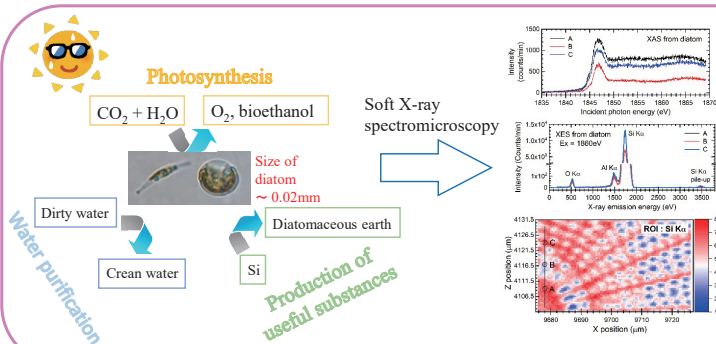
As go through the periodic table from left to right, it is observed that the valence of transition metal decreases, that of lead increases, and the charge distribution changes systematically



Reference: Y. Sakai *et al.*, *J. Am. Chem. Soc.* 139, 4574 (2017)

Eco-friendly diatoms

- Visualized the elemental and chemical-state distributions in the frustule of *Arachnoidiscus* sp.
- Developing applications for oxygen gas, water purification, bio-fuels, etc.



We observed the frustule of *Arachnoidiscus* sp. by using soft X-ray spectromicroscope, and succeeded in the visualization of

- elemental distribution, and
- chemical-state distribution.

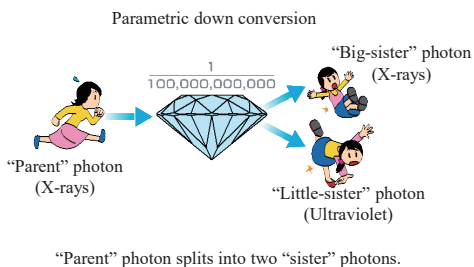
From now on, we will aim at observing cell nucleus, chloroplast as well as lipid of living diatoms. We will also study the formation of the frustule and also the distribution of chloroplast in the diatoms.



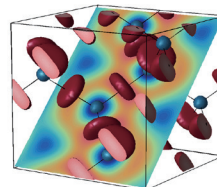
Oura, Ishihara *et al.*, in preparation

Observing details beyond the limits of wavelengths

- Use of parametric down conversion breaks the barriers of diffraction limits
- Visualizing optical responses at any wavelength at atomic resolution



Spatial resolution reaches $1/380$ wavelength



Optical response of diamonds to 20.7-nm ultraviolet is revealed with 0.054-nm atomic resolution.

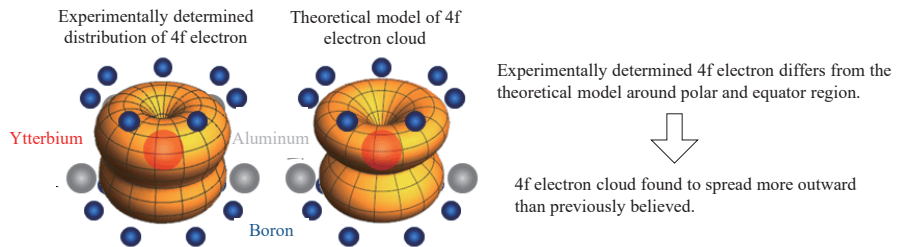


Reference: K. Tamasaku *et al.*, *Nat. Phys.*, **7**, 705 (2011)

■ Observing electron clouds inside solids

- Visualized the spatial distribution of 4f electrons for an ytterbium compound
 - Determined that the 4f electron spreads outward along the neighboring boron atoms
- Observing electron clouds to facilitate the development of innovative properties in solids

4f electron cloud investigated by HAXPES

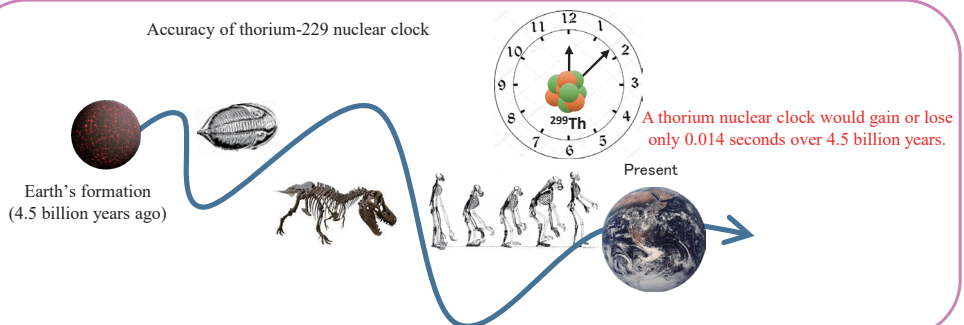


Reference: K. Kuga *et al.*, *Phys. Rev. Lett.*, **123**, 036404 (2019)

■ Developing an ultra-precise nuclear clock

- Successful X-ray pumping of thorium-229 into the metastable excited (isomer) state
- Paving the way for a “nuclear clock”, which would be much more accurate than current cesium-based atomic clocks

Accuracy of thorium-229 nuclear clock

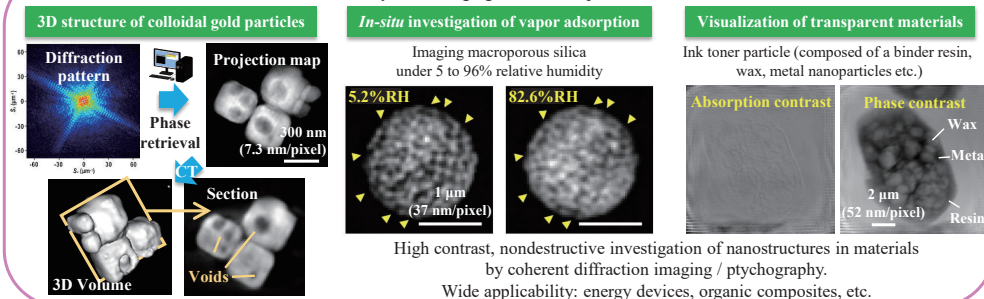


Reference: T. Masuda *et al.*, *Nature*, **573**, 238 (2019)

Visualizing materials that are invisible to electron microscopes

- A combination of coherent X-rays and computational imaging methods extends the spatial resolution of X-ray microscopy from several tens of nano-meters to less than 10 nm
- X-rays allow investigation of internal structures under moist/redox gas atmosphere
→ Providing a method for nano-structural analysis of thick materials for industrial fields

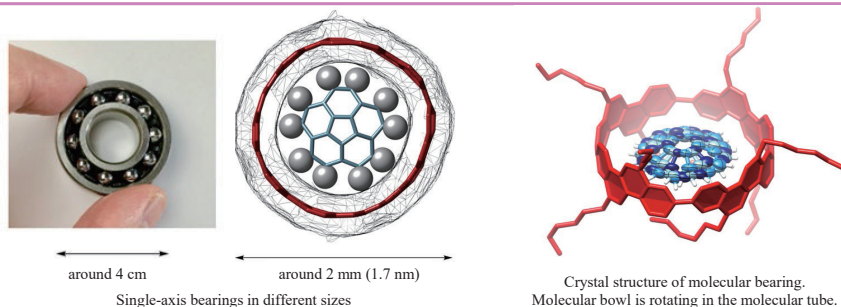
Lensless X-ray nano-imaging under atmospheric condition



Reference: Y. Takayama *et al.*, *J. Synchrotron Rad.*, **25** (4), 1229 (2018)

Nanometer-sized molecular bearings rotating around a single axis

- Encapsulated a molecular bowl within a 2-nm molecular cylinder *via* multiple CH- π hydrogen bonds
- Arranged ten weak hydrogen bonds in concyclic arrays allow for single-axis rotations
→ Developing new molecular machines with innovative rotational mechanisms

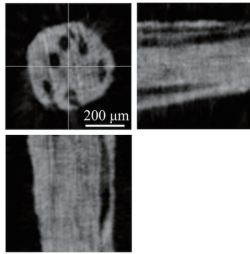


Reference: T. Matsuno *et al.*, *Nat. Commun.*, **9**, 3779 (2018)

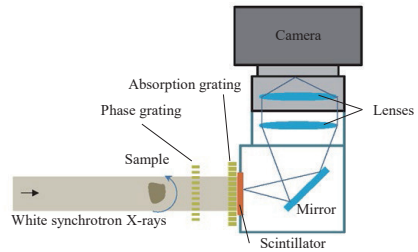
A world record for high-speed 3D imaging

- Achieved the world's fastest X-ray CT of organic materials within milliseconds with a spatial resolution of about 20 μm
- Achieving ultrafast 4D (spatial 3D + temporal) observation capabilities

Ultrafast X-ray CT was performed using a grating-based X-ray interferometry with white synchrotron X-rays



CT images of a piece of wood with a measurement time of 4.43 ms



Experimental setup of X-ray grating interferometer for millisecond-order X-ray phase tomography using fringe scanning method

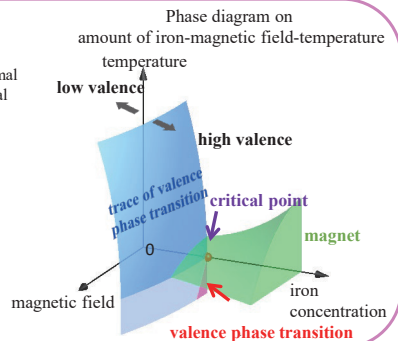
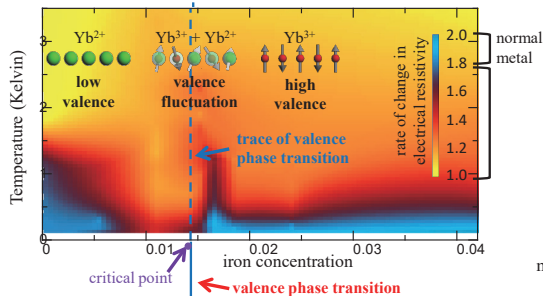


Reference: W. Yashiro *et al.*, *Appl. Phys. Express*, **10**, 052501 (2017)

Innovative Superconducting State

- Discovered an anomalous metal that has a unique electron state and quantum valence fluctuation
- Developing devices with greater energy efficiency

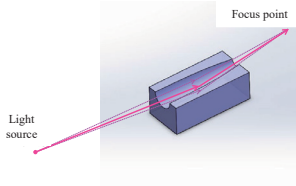
Metallic state with respect to iron concentration and temperature



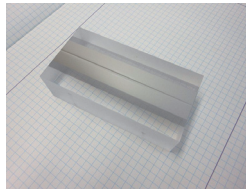
Reference: K. Kuga *et al.*, *Science Advances*, **4**, eaao3547 (2018)

- A two-dimensional ellipsoidal mirror with nanometer precision
 - Achieved a world record focus size of 100 nm using a single ellipsoidal mirror
 - Developing future applications using nano-focus beams in X-ray microscopes

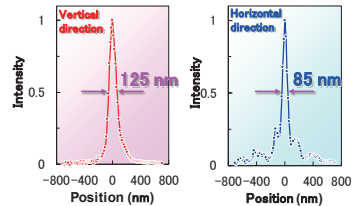
Formation of two-dimensional focused beam using a single ellipsoidal mirror



Photograph of ellipsoidal mirror



Intensity profile of x-ray focused beam using ellipsoidal mirror



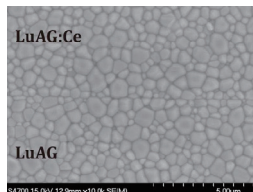
World record of 100 nm focus size



Reference: H. Yumoto *et al.*, *Sci. Rep.*, **7**, 16468 (2017)

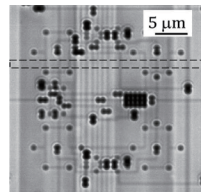
- X-rays with a resolution close to the theoretical limit
 - Developed an X-ray imaging device with high optical properties
 - Demonstrated visualization of a 200 nm structure
 - Enabling non-destructive inspection of semi-conductor integrated circuits with minute wiring

X-ray scintillator inside x-ray camera (left) and its enlarged image (right)



Fully densified crystals without voids suppresses light diffusion and enhance optical property

X-ray transmission image of very large-scale integration circuit



Successfully visualized 300 nanometer width aluminum wiring lines

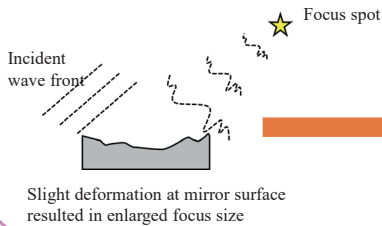


Reference: T. Kameshima *et al.*, *Opt. Lett.*, **44**, 1403 (2019)

A mirror for the world's smallest X-ray focused beam

- Developed a technique for modulating X-ray wavefronts using a deformable mirror
- Enabling further technical development for achieving smaller X-ray focused beams

Focus size limited even by world's most precisely fabricated mirror



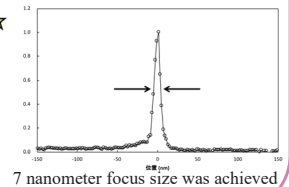
Deformable mirror to modulate wave front



Piezo Electric Element

Incident wave front

X-ray focus beam in nanometer size realized by modulating incident wave front



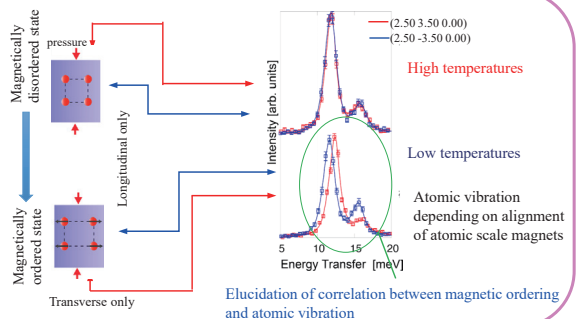
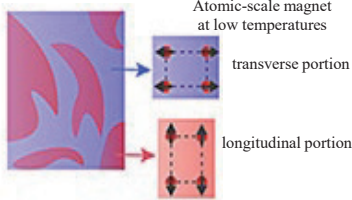
Reference: H. Mimura *et al.*, *Nat. Phys.*, **6**, 122 (2010)

Mechanisms of innovative superconductors

- Elucidating superconducting mechanisms using cooperating atomic motion and atomic scale magnets
- Designing new materials to increase energy efficiency for electronic power supply and storage plants to keep surplus power

SrFe_2As_2

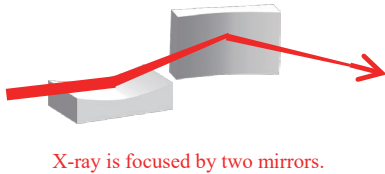
(A model material of superconductor)



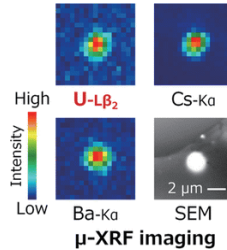
Reference: N. Murai *et al.*, *Phys. Rev. B* **93**, 020301(R) (2016)

- Development of a focusing mirror for more intense and smaller X-rays
 - Focusing X-rays with mirrors
 - Observing the state of atmospheric dust identified to have originated in a nuclear power plant
 - Enabling applications for various experiments

X-ray focusing optics (K-B Mirrors)



Analysis of atmospheric dust



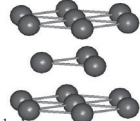
This particle was identified to be from the nuclear reactor!



Reference: Y. Abe *et al.*, *Anal. Chem.*, **86**, 8521(2014)

- Discovering magnetism under high pressure
 - Revealed modifications to the atomic arrangement and magnetism of cobalt by applying a high pressure of 100 GPa
 - Revealed the stability of new paramagnetic states of cobalt, contradicting the theoretical predictions of strong magnetism disappearing
 - Discovering new relationships between pressure and magnetism

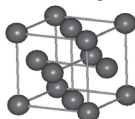
Atomic arrangement at ambient pressure



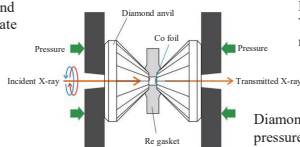
Hexagonal close-packed (hcp) structure and ferromagnetic state



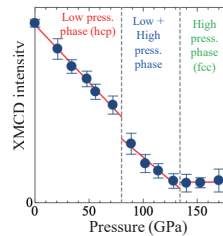
Atomic arrangement at 100 GPa



Face-centered cubic (fcc) structure, Theory predicts the system goes to non-magnetic state



Diamond anvil cell is used to generate pressure higher than 100 GPa.



The experimental result show that Co keeps to be magnetic in another paramagnetic state.

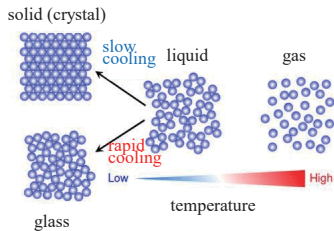


Reference: N. Ishimatsu *et al.*, *Phys. Rev. B* **83**, 180409 (2011)

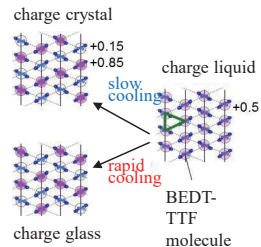
A glass-forming charge liquid

- New insights into the behavior of electrons as liquids transform to glass, deepening our understanding of this transition phase
- Understanding the universal nature of the liquid-glass transition

Slow cooling of liquids causes a crystallization of atoms into solid. However, when the material was cooled quickly, crystallization was avoided and turning into glass state with no long-range periodicity.



Unique glassy state of π -electrons on the triangular lattice in an organic molecular conductor was found after rapid cooling.



Reference: S. Sasaki *et al.*, *Science*, **357**, 1381 (2017)

Unraveling the complex phenomena in many-body systems

- Used optical spectroscopy to reveal the behavior of electrons in a triangular relationship
- Answering the question of why electron spins behave like liquids

Electrons form or don't form pairs. Each state has almost the same energy and changes dynamically even at very low temperatures.

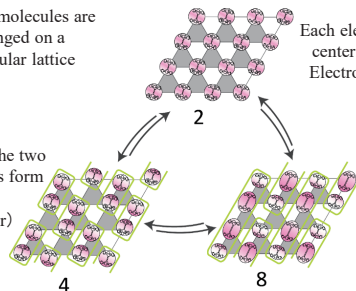


Electron spins behave like liquids.

An approach to many-body problems which cannot be solved by analytical calculation

Pairs of molecules are arranged on a triangular lattice

Electrons in the two closest circles form a pair (Tetramer)



Each electron is located at the center of a different circle. Electrons do not form pairs (Dimer)

Two electrons form a pair in a long ellipse (Octamer)

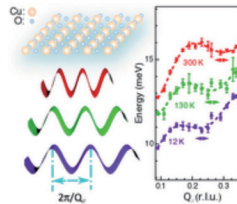
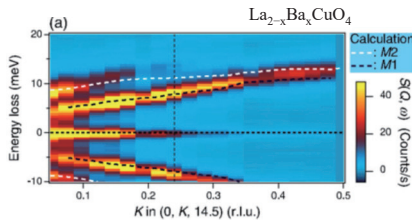


Reference: T. Yamamoto *et al.*, *Sci. Rep.*, **7**, 12930 (2017)

Unveiling the mechanisms of high-temperature superconductors

- Measured the lattice vibrations of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ with high precision to clarify the correlation with charge density waves
- Providing clues for the development of new superconducting materials

Measured phonon spectra interacting with charge density waves (CDWs)



CDW periodicity shift depending on temperature

Comparison with other high temperature superconducting material $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$

Both materials have common origin of CDW instability.

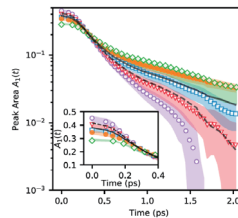
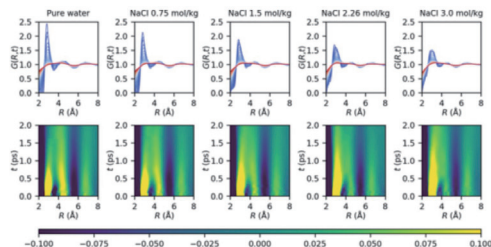


Reference: H. Miao *et al.*, *Phys. Rev. X*, 8, 011008 (2018)

Ion dynamics in a water solution

- Investigated NaCl solution dynamics at sub-nanometer, sub-picosecond scales
- Clarified the local structures of water molecules and Na^+ and Cl^- ions, and their time dependences
- Understanding aqueous chemical reactions at the atomic scale

Concentration dependent time-space correlation function $G(R,t)$ of NaCl solution



The first step for visualization of atomic scale chemical reactions in water solution



Reference: Y. Shinohara *et al.*, *Phys. Rev. Materials*, 3, 065604 (2019)

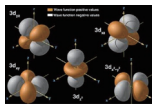
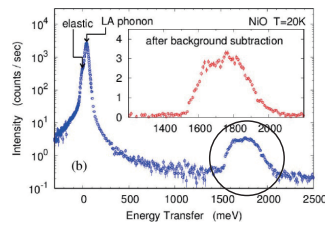
Observing electron orbitals

- Investigated the electronic excitations of NiO under d-orbitals (*d-d* excitation)
- Clarifying the relationship with electronic orbitals and physical properties and understanding the local extent and non-uniformity of electronic orbitals

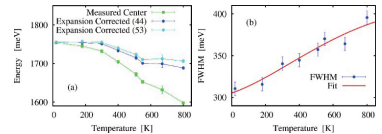
Crystal structure of NiO



3d-orbitals

*d-d* excitation in NiO

Direct observation of scattered x-rays from 3d-orbitals

Temperature dependence of *d-d* excitation in NiO

The change of lattice vibration and magnetism sensitively reflects to electronic orbitals

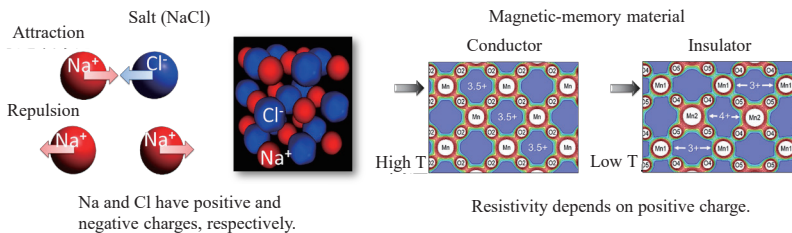


Reference: D. Ishikawa *et al.*, *J. Phys. Soc. Jpn.* **86**, 093706 (2017)

Development of new electronic devices

- Developing a tool for visualizing the interactions between atoms
- Understanding electrical properties and crystal structures

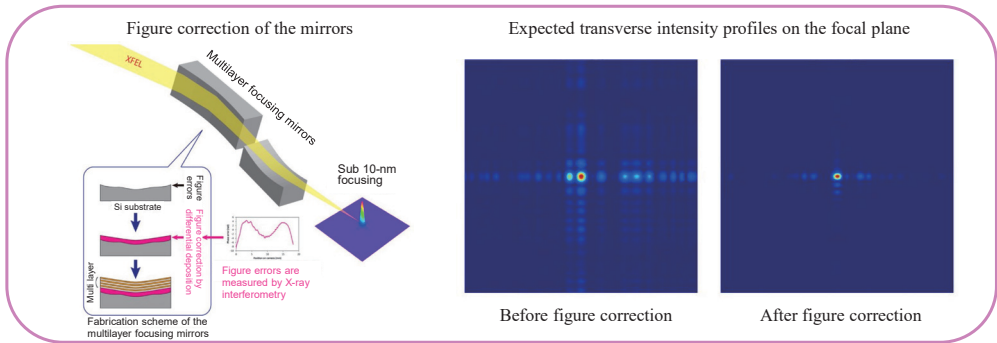
Visualizing interactions between atoms



Reference: K. Kato *et al.*, *Adv. Phys.: X* **1**, 55 (2016)

Ultimate focusing of an X-ray laser beam

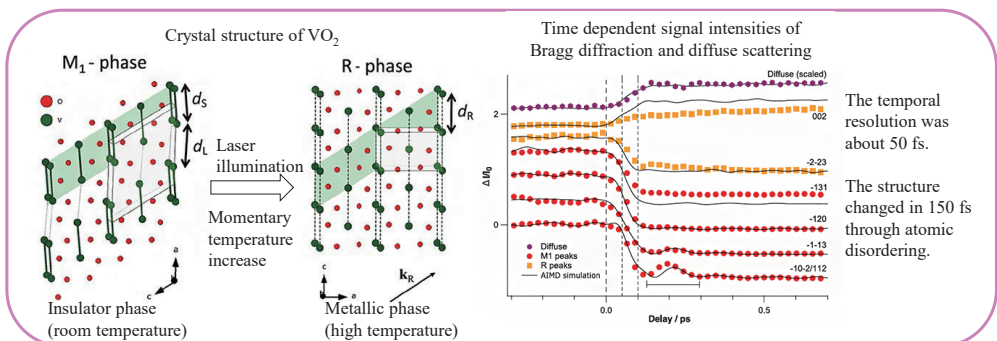
- Fabricated X-ray focusing mirrors with steep surface profiles through characterization by X-ray interferometry and differential deposition
- Focused an X-ray laser beam into a sub 10-nm spot
- Achieving an important milestone in the development of single-molecular imaging



Reference: S. Matsuyama *et al.*, *Sci. Rep.*, **8**, 17440 (2018)

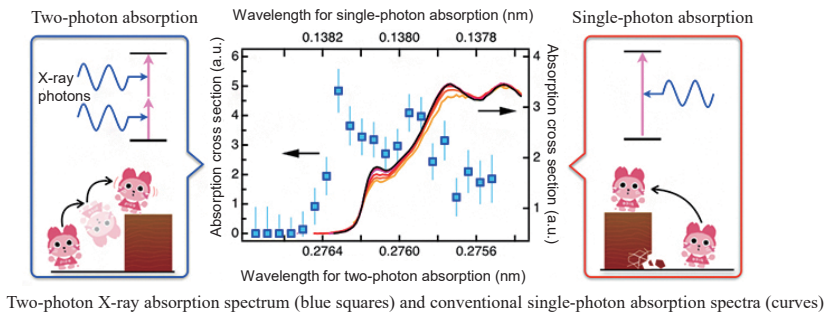
Mechanism for light-induced insulator-to-metal transition

- Observed an ultrafast process of light-induced insulator-to-metal transition
- Found that the transition is driven by atomic disordering, unlike in the conventional model
- Establishing new techniques that use light to control material properties



Reference: S. Wall *et al.*, *Science*, **362**, 572 (2018)

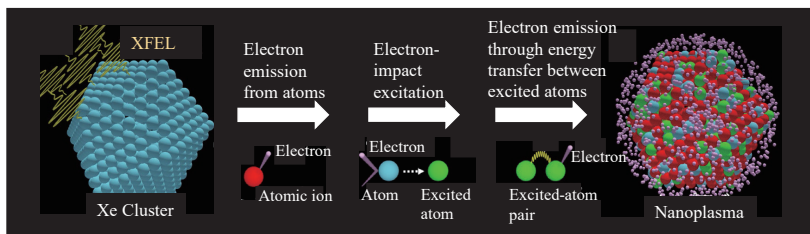
- Foundation for X-ray optical physics in the 22nd century
 - Demonstration of a new spectroscopic technique using simultaneous two X-ray photon absorption
 - Providing useful information about transition-metal *d* orbitals, which play important roles in exotic devices such as high temperature superconductors



Reference: K. Tamasaku *et al.*, *Phys. Rev. Lett.*, **121**, 083901 (2018)

- Intense XFEL can change materials into extreme states
 - Created nanoplasma from a Xe cluster using XFEL irradiation
 - Revealed experimentally and theoretically the mechanisms of nanoplasma formation
 - Enabling fine control of plasma through better understanding their formation mechanisms

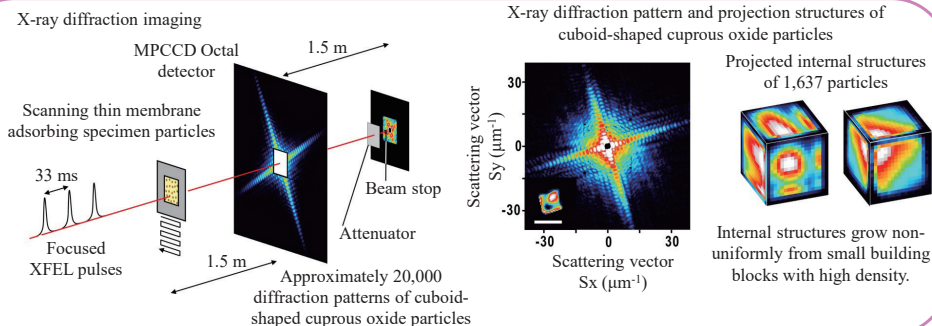
The mechanism of nanoplasma formation in a Xe cluster



Reference: Y. Kumagai *et al.*, *Phys. Rev. X* **8**, 031034 (2018)

Visualizing the internal structures of nano-sized metal particles

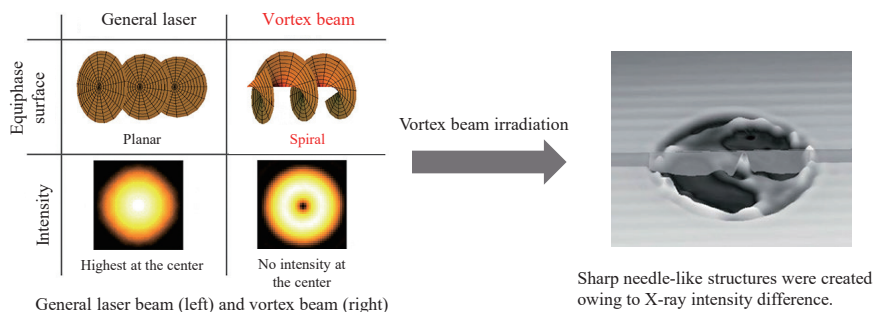
- Visualized the structures of nano-particles, which are expected to open new technologies in medical and engineering fields
 - Found that internal structures change in the growth of cuboid-shaped cuprous oxide particles
- Developing a new methodology for nano-particle synthesis



Reference: T. Oroguchi *et al.*, *Nano Lett.*, **18**, 5192 (2018)

Microfabrication using an X-ray vortex

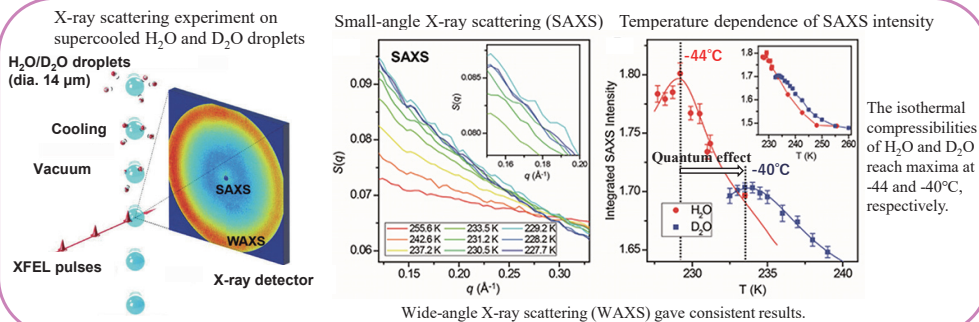
- Produced an optical vortex in the hard X-ray region
 - Applied the X-ray vortex to the fabrication of needle-like structures smaller than the X-ray beam size
- Developing a new microfabrication technique with element selectivity



Reference: Y. Kohmura *et al.*, *Appl. Phys. Lett.*, **112**, 123103 (2018)

Revealing the secrets of water

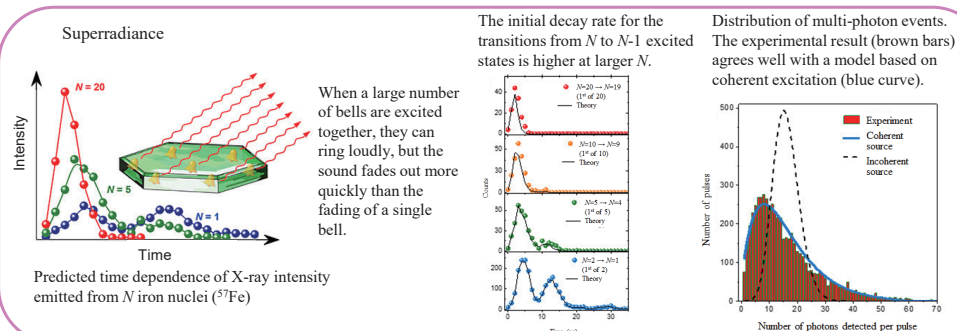
- Explored the thermodynamic properties of super-cooled water
- Demonstrated the existence of a critical point for liquid-liquid transition
→ Understanding the origins of the unique thermodynamic properties of water



Reference: K. H. Kim *et al.*, *Science*, **358**, 1589 (2017)

Verifying important theories of physics

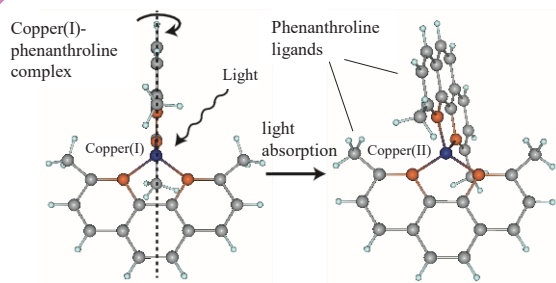
- Observed nuclear super-radiance, a quantum mechanical phenomenon originally predicted in 1954
→ Providing fundamental information for interpreting the results of XFEL experiments



Reference: A. I. Chumakov *et al.*, *Nat. Phys.*, **14**, 261 (2018)

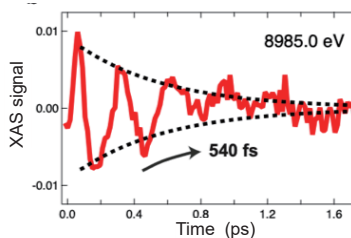
Ultrafast oscillation of molecules

- Observed the oscillation of a metal complex upon light absorption with a high spatiotemporal resolution
- Succeeded in recording a “molecular movie” during the photoreaction
- Contributing to the development of photocatalysts and artificial photosynthetic systems through a better understanding of photoreaction mechanisms



The dihedral angle between the ligands reduces from 90° to $\sim 70^\circ$.

Molecular oscillations were observed on a femtosecond timescale by X-ray absorption spectroscopy (XAS).



Reference: T. Katayama *et al.*, *Nat. Commun.*, **10**, 3606 (2019)

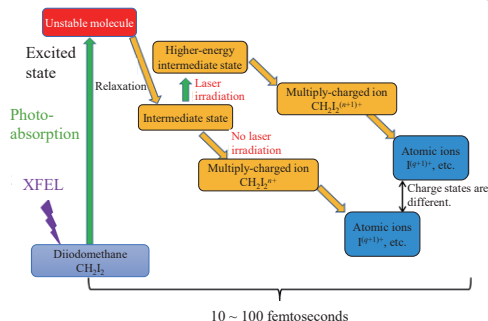
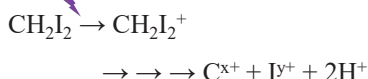
Understanding the mechanisms of radiation damage

- Observed ultrafast relaxation processes in molecules after they absorbed X-rays
- Demonstrated a technique for revealing the mechanisms of X-ray induced damage of molecules
- Contributing to the development of cancer radiotherapy

Ultrafast molecular dissociation after XFEL irradiation was observed by using a pump-and-probe technique.

The temporal resolution of a few tens of femtoseconds was achieved owing to ultrashort XFEL pulses of SACLA.

X-ray free-electron laser

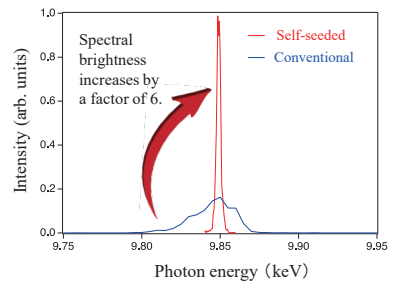
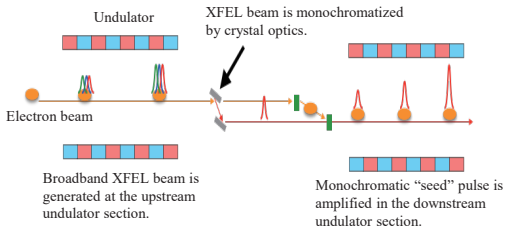


Reference: H. Fukuzawa *et al.*, *Nat. Commun.*, **10**, 2186 (2019)

More brilliant XFEL

- Developed a new optical scheme “reflection self-seeding” to generate brighter XFEL
- Achieved a spectral brightness six times more intense than conventional XFEL
- Providing new opportunities for research using SACLA's facilities

Reflection self-seeding

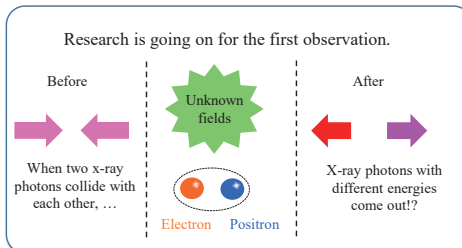


Reference: I. Inoue *et al.*, *Nat. Photon.*, **13**, 319 (2019)

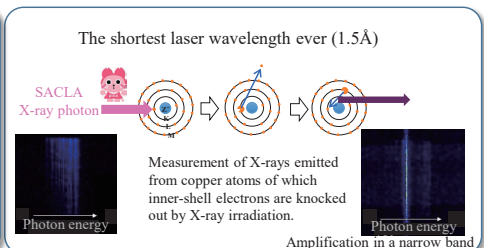
Exploring new phenomena

- Meeting the challenge of observing unknown fields
- Developing an atomic laser with the shortest wavelength to-date
- Opening new scientific fields for research and discovery

Search for unknown fields through photon collision experiments



Laser using a inner-shell level of copper

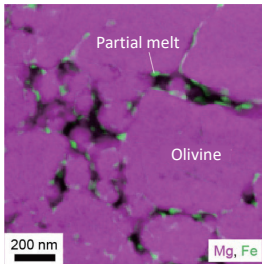


Reference: T. Inada *et al.*, *Phys. Lett. B* **732**, 356 (2014)
H. Yoneda *et al.*, *Nature*, **524**, 446 (2015)

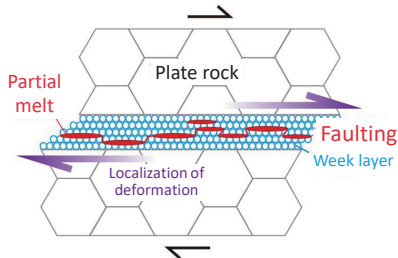
Origin of earthquakes deep within the Earth

- Monitoring micro-earthquakes that radiate from a deforming rock at high-pressure and high-temperatures in subducting oceanic plates
- Revealed the origin of earthquakes to be the partial melting of rocks due to the localization of deformation energy
- Revealing new insights for the mechanisms causing intermediate-depth and deep earthquakes

Quenched partial melt (glass) in a fault zone



Faulting triggered by localized deformation in rocks

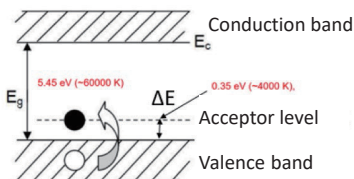


Reference: Ohuchi *et al.*, *Nature Geoscience*, **10**, 771 (2017)

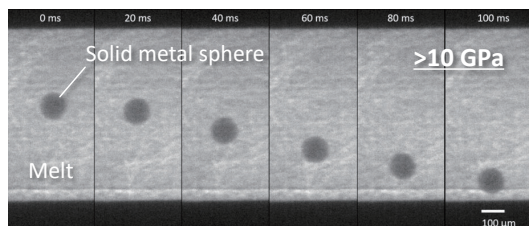
Developing high-performance furnaces that are X-ray-transparent

- Developed a semiconductor heater made of boron-doped diamonds capable of generating 4000 K at high-pressure conditions
- Measured the viscosities of silicate melt under pressure
- Exploring material differentiations in the molten and chilling conditions early in Earth's history

Band structure of diamond



Falling sphere in a molten silicate. Viscosities of melt were evaluated by the falling velocities of solid sphere.

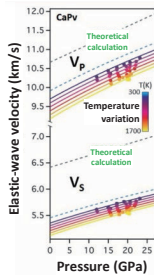


Reference: Xie *et al.*, *Rev. Sci. Instrum.*, **88**, 093904 (2017)

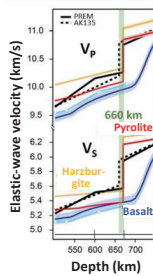
Fate of the subducted ocean crust deep in the Earth's interior

- Determined that residual former oceanic crusts can exist at the top of the lower mantle by using high-pressure/temperature *in situ* sound velocity measurements on a calcium-rich mineral material
- Exploring the structural and chemical composition of the Earth's mantle to constrain mechanisms of mass transport by convective systems

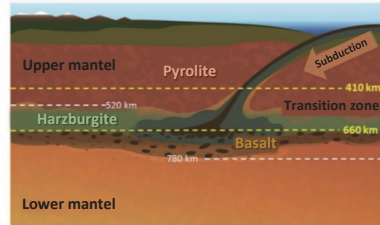
Elastic-wave velocities of CaSiO_3 perovskite



Elastic-wave velocities of model rocks in the mantle



Chemical composition and structure of the Earth's mantle across the 660-km discontinuity

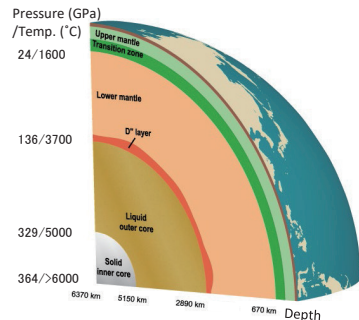
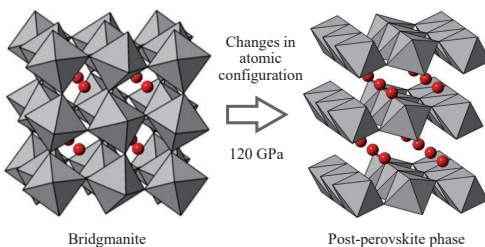


Reference: Gréaux *et al.*, *Nature*, **565**, 218 (2019)

Earth's deep interior and its evolution

- Discovered a new high-pressure phase for magnesium silicate perovskite using innovative experiments that mimic conditions at the core-mantle boundary
- Succeeded in making *in situ* X-ray observations under high-pressure and high-temperature extreme conditions corresponding to the center of the Earth
- Understanding the structures and dynamics of the Earth's deep interior

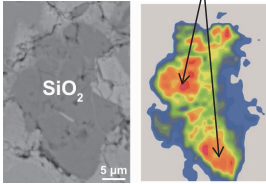
Phase transition in MgSiO_3 silicate



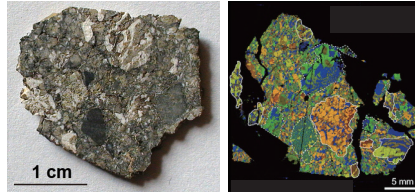
Reference: M. Murakami *et al.*, *Science*, **304**, 5672 (2004)
S. Tateno *et al.*, *Science*, **330**, 6002 (2010)

- Exploration the potential of space resource mining in the near future
 - Analyses of a lunar meteorite revealed a mineral that typically indicates traces of frozen water.
 - Understanding the nature and quantity of water on the surface of the moon

Moganite, a mineral that requires the presence of water to form

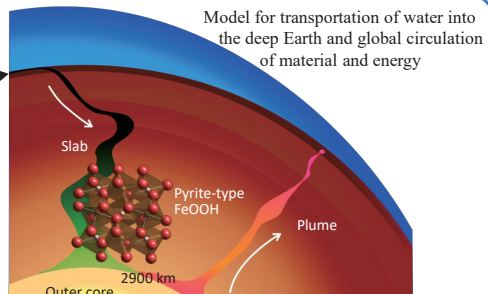
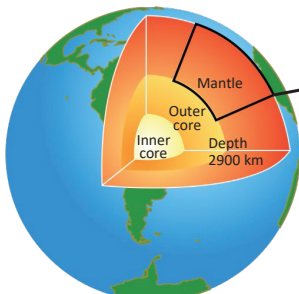


Lunar meteorite NWA2727 which has originated from the Lunar Procellarum basin



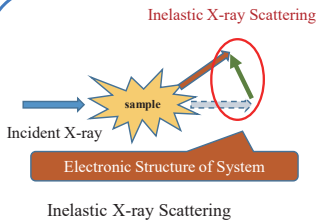
Reference: M. Kayama *et al.*, *Sci. Adv.*, **4**, eaar4378 (2016)

- Ocean sustainability and the Earth's deep interior
 - Proposing stable water-transportation into the lowermost mantle from the surface
 - Increasing our understanding of deep water cycles, including the spatial variability and temporal stability of water storage deep within the Earth

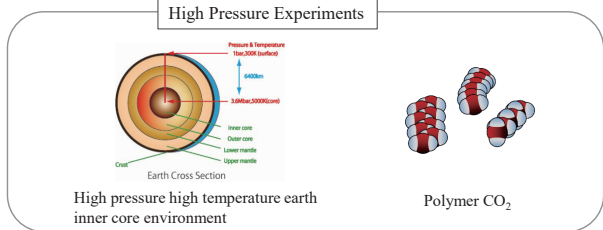


Reference: M. Nishi *et al.*, *Nature*, **547**, 205 (2017)

- Investigation of electronic properties of the Earth's inner core environment
 - High pressure inelastic X-ray scattering
 - Polymer CO₂ under pressure
- Studying electronic structures under extreme conditions



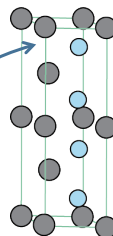
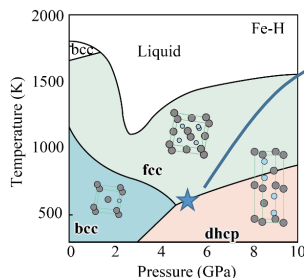
Large penetration depth and high brilliant synchrotron light x-ray allowed to investigate small confined area of sample environment.



Reference: Nomura *et al.*, *Nature*, **473**, 7346 (2011)
S.R. Shieh *et al.*, *Proc Nat. Acad. Sci.*, **110**, 18402 (2013)

- Possible presence of noble iron hydride in Earth's interior
 - Synthesized Iron hydride FeH_x under high temperature-pressure (*T-P*) conditions
 - Found hydrogen atoms partially occupying the interstitial sites of iron metal lattices
- Estimating the hydrogen content of the inner core of the Earth

The pressure-temperature phase diagram previously reported for the iron-hydrogen system



The occupation sites of hydrogen atoms in the hexagonal closed-pack metal lattice was determined by synchrotron radiation x-ray and neutron diffraction measurements. Gray and light blue circles represent iron and hydrogen atoms, respectively.

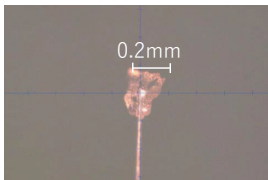


Reference: A. Machida *et al.*, *Sci. Rep.*, **9**, 12290 (2019)

Origin of the Itokawa asteroid

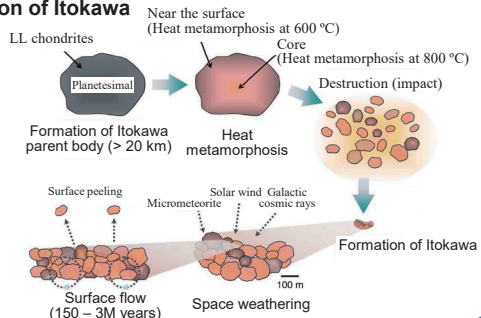
- Analyzed the atomic arrangement of the Itokawa asteroid
- Clarified the formation process of Itokawa using a combination of several techniques
- Applying learnings to the Hayabusa 2 space mission

Itokawa dust particle retrieved by Hayabusa



- ✓ What substances does Itokawa consist of?
- ✓ How Itokawa was born?

Formation of Itokawa

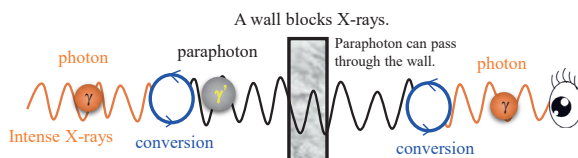


Reference: T. Nakamura *et al.*, *Science* **333**, 1113 (2011)

Searching for hidden elementary particles

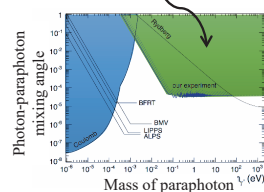
- Experimental detection of hidden elementary particles that have been predicted by theory
- Excluding a large parameter range for paraphotons

Light shining through a wall experiment



X-ray photons could be converted to paraphotons that pass through the wall.

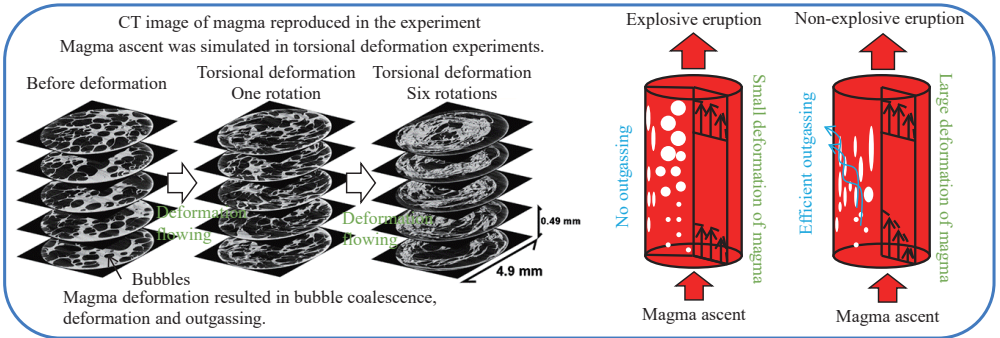
Rejected area of paraphoton by this research



Reference: T. Inada *et al.*, *Phys. Lett. B* **722**, 301 (2013)

Dynamics of volcanic eruptions

- Simulating the ascent of magma to the Earth's surface in a laboratory and observing it with *in situ* X-ray micro-CT
 - Determining the mechanisms of outgassing from magma and their rates
 - Clarifying parameters that control the bifurcation between explosive and non-explosive states
- Contributing to better predictions of the explosivity of volcanic eruptions

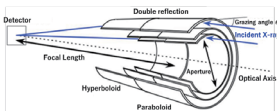


Reference: S. Okumura *et al.*, *EPSL*, **362**, 163 (2013)
S. Okumura *et al.*, *JGR*, **120**, 10.1002/2014JB011532.(2015)
M. Kameda *et al.*, *Sci. Rep.*, **7**, 16755 (2017)

Exploring the mysteries of cosmic particle accelerators

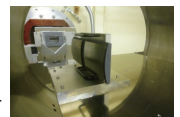
- Developed an X-ray telescope to investigate the acceleration mechanisms of high-energy particles (cosmic rays) traveling in outer space
- Observing the high-energy X-rays emitted at the birth of cosmic rays

Hard X-ray telescope (HXT) for ASTRO-H satellite launched in 2016



Unfortunately, ASTRO-H became inoperable two months after launch. However, a balloon experiment called XL-Calibur project is in progress using the developed systems.

A FORCE project to elucidate the growth of black holes is also in progress. NASA, Osaka University, Ehime University and University of Miyazaki etc. are jointly developing an HXT with improved angular resolution.

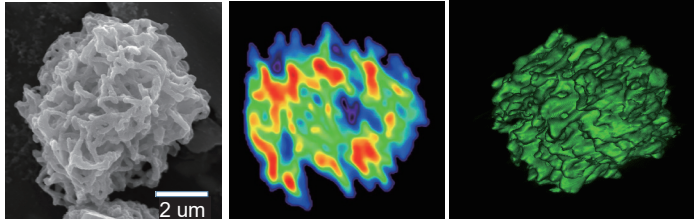


Reference: H. Awaki *et al.*, *Applied Optics*, **53**(32), 7664 (2014)
H. Matsumoto *et al.*, *J. Astron. Telesc. Instrum. Syst.*, **4**, 011212 (2018)
H. Mori *et al.*, *J. Astron. Telesc. Instrum. Syst.*, **4**, 011210 (2018)

Discovery of abundant Mn-microparticles from deep-sea oxic sediments

- Used nano-computed tomography (nano-CT) to identify the shape and microstructure of ferromanganese mineral microparticles, discovered within deep-sea oxic sediments
- Discovered a global source for manganese within Mn-microparticles that is comparable to the supply of on-land manganese ores
- Clarifying the formative relationships between Mn-microparticles and deep-sea Mn-mineral resources (Mn-nodules and -crusts)

High-resolution images of Mn-microparticles separated from deep-sea sediments
SEM image Cross-sectional and 3D images taken by nano-CT



⇒ Mn-microparticles consist of tangled fibrous ferromanganese minerals without core material or concentric growth structure

Chemical composition of Mn-microparticles is similar with that of deep-sea Mn mineral resources, but shape and microstructure of the microparticles are different from the mineral resources.



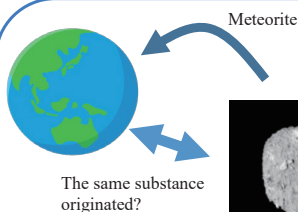
Mn-microparticles can provide critical information for the primary processes in formation of deep-sea Mn mineral resources.



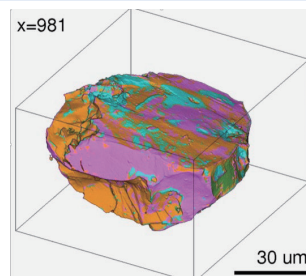
Reference: G. Uramoto, Y. Morono *et al.*, *Nat. Commun.*, **10**, 400 (2019)

Comparison of meteorites to extraterrestrial materials

- Revealed that meteorites discovered on Earth originate from asteroids
- Understanding better the evolution of the solar system based on the relationships between materials that make up the Earth and extraterrestrial materials



S-type asteroid "Itokawa"



3D CT image of mineral distribution of Itokawa particle. Mineral and chemical composition are consistent with meteorites discovered on earth.



Reference: A. Tsuchiyama *et al.*, *Science*, **33**, 1121 (2011)

A new exotic particle, “Pentaquark”

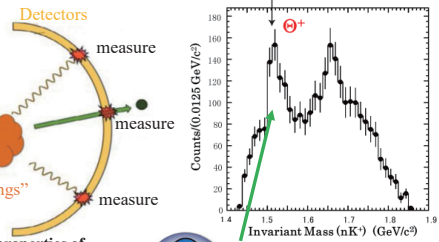
- Found a new particle Θ^+ (pentaquark :Theta⁺) using a Laser-Electron Photon beam while exploring the world of quarks, the ultra-tiny particles that constitute matter

BL31LEP
BL33LEP

“Watch” the smallest world with Laser-Electron Photons

High energy electrons of SPring-8
Laser-Electron Photons
Target
hit the target
“unknown things” are produced
High intensity Laser-Electron Photons are generated
(1 million times the energy of X-rays)

How to know the masses and properties of unknown particles
→ measure emitted nucleons and mesons from their decays



Existence of a new exotic particle which consists of 4 quarks and an anti-quark was suggested



Reference: T. Nakano *et al.*, *Phys. Rev. C* **79**, 025210 (2009)
Y. Kato *et al.*, *Few. Body Syst.*, **54**, 1245 (2013)

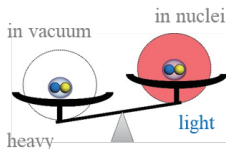
Approaching the source for the mass of objects

- Exploring the origin of mass by creating mesons in nuclei using a Laser-Electron Photon beam and measuring the changes of their mass

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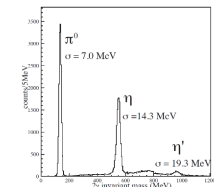
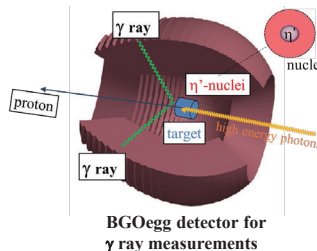
Mystery of Mass:

A proton consisting of three quarks is about 100 times heavier than the sum of three quarks!



The meson mass is expected to become lighter at high density or high temperature
→ to elucidate the origin of mass

produce η' meson in nuclei with high density by irradiating the Laser-Electron Photon beam to the target, and measure its mass by investigating its decay (η' meson is the heaviest member in the congener of π meson)



Example of the measurement of meson masses from two γ rays

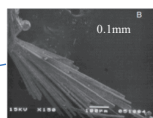
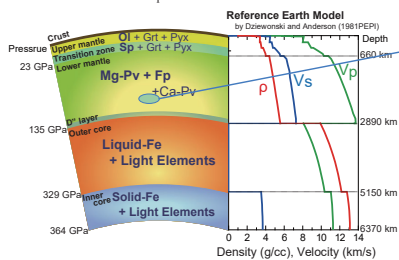


Reference: N. Muramatsu *et al.*, *Phys. Rev. C* **100**, 055202 (2019)

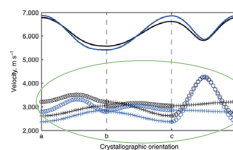
Nature of seismic waves

- Observation of anisotropic elastic constants in the model material isostructural with rocks deep within the Earth
 - Observation of place dependence of seismic speed below the Earth's surface
- Elucidating the correlation between the alignment of rocks and the propagation of seismic waves

Inside structure of the earth and propagation of seismic waves (V_p and V_s)



Simulated bedrock having the same crystal structure as the rocks deep in the earth



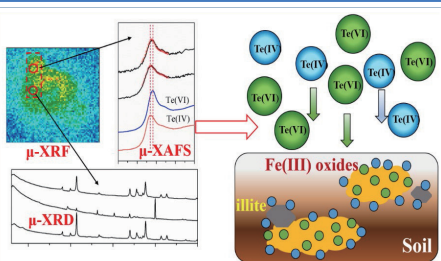
Successfully reproduce propagation of seismic waves depending on the alignment of rocks



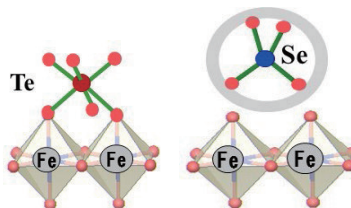
Reference: A. Yoneda et al., *Nat. Commun.*, **5**, 3453 (2014)

Environmental behavior of a useful but toxic rare metal, tellurium (Te)

- Revealed that inner-sphere complexation with iron (Fe) oxides is a primary important factor for determining the environmental behavior of Te
 - Revealed a relation between the difference of Te from its congener, selenium (Se), and the acidity of the two ions
- Finding applications for safer use of rare metals



Factors controlling behavior of Te at earth's surface was clarified by micro(nano)-XRF-XAFS-XRD method.



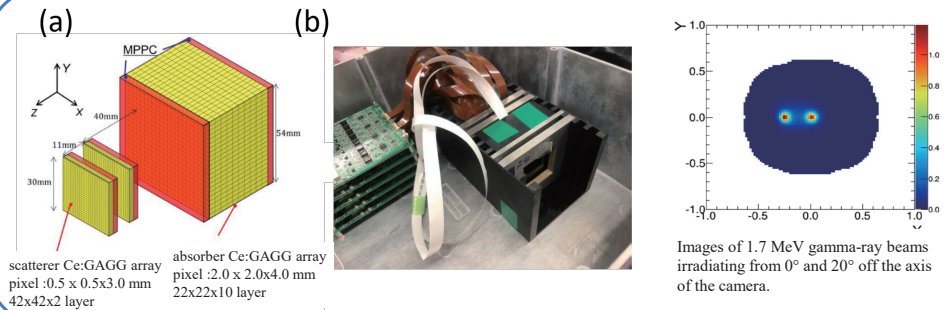
Te forms insoluble inner-sphere complex to Fe oxides, but Se soluble outer-sphere complex.



Reference: H. Qin et al., *Environ. Sci. Technol.*, **51**, 6027 (2017)

Exploring the universe with gamma rays

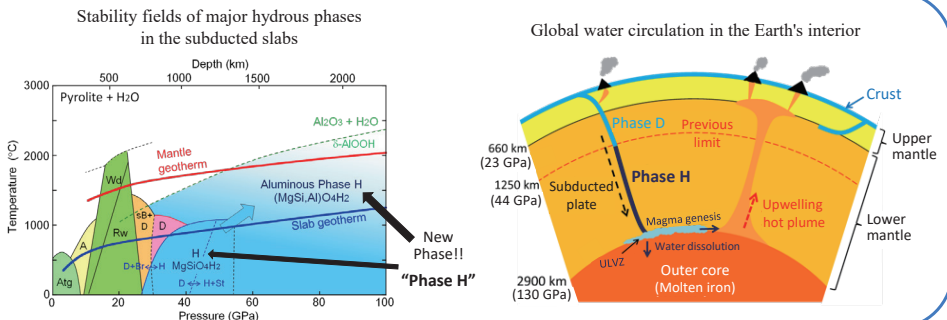
- Developed an ultra-compact MeV gamma ray camera
- Providing new eyes to explore the universe



Reference: H. Hosokoshi *et al.*, *Sci. Rep.*, 18551 (2019)
<https://www.nature.com/articles/s41598-019-54862-z>

Predicting the Earth's future based on global water cycling

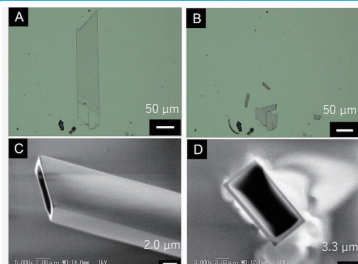
- Found a new hydrous mineral “phase H” to be stable up to the core-mantle boundary, implying that water is transported into the core through the thick mantle
- Understanding the effects of deep water and its circulation and how it has shaped the Earth's evolution



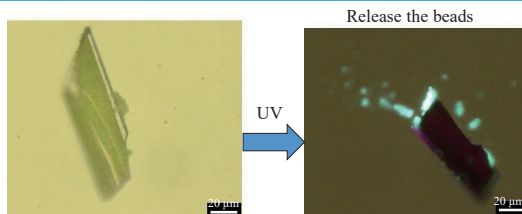
Reference: M. Nishi *et al.*, *Nature Geoscience*, 7, 224 (2014)

A photo-induced release system using hollow crystal capsules

- Discovered hollow crystals that show photosoluble phenomena and their mechanisms
- Found that UV exposure induces cracking of the hollow crystals packed with beads
- Developing a light-induced release system that mimics Impatiens in nature



Optical microscopic images of hollow crystal (A) before UV exposure, (B) after exposure and (C, D) SEM images of hollow crystal



Hollow crystal packed with fluorescent polystyrene beads scatter the beads by the UV irradiation like the behavior of hollow-structured Impatiens in nature.

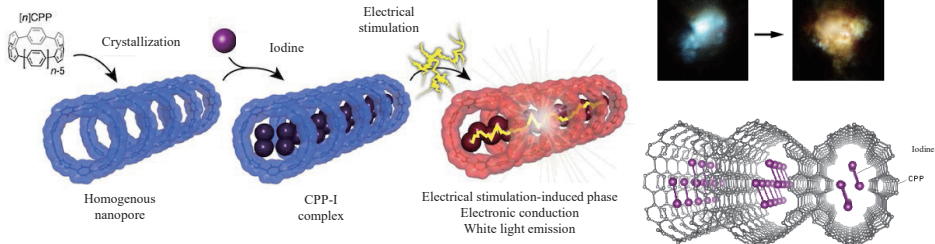
Figures are provided by Ryukoku Univ.

Reference: E. Hatano *et al.*, *Angew. Chem. Int. Ed.*, **56**, 12576 (2017)

New functional materials for artificial muscles

- Applying electrical stimulation to develop materials with electronic conductivity and unique light-emission features
- Observed structural changes during electrical stimulation using *in situ* measurements
- Developing innovative technology such as drug delivery systems and next-generation lighting devices

Entrapping functional molecules in nano-space

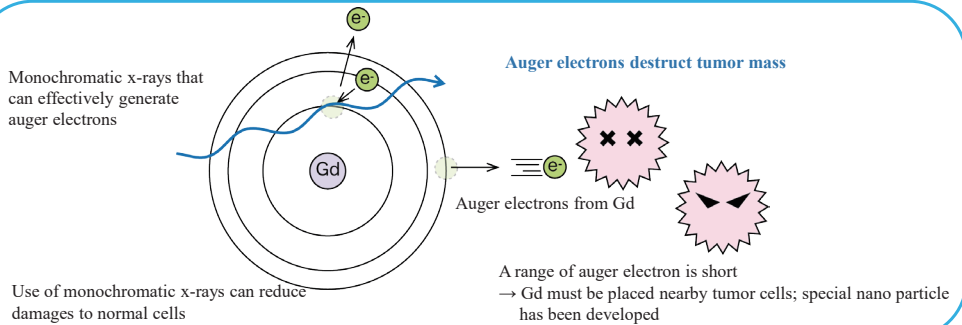


Light emission due to electrical stimulation

Reference: N. Ozaki *et al.*, *Angew. Chem. Int. Ed.*, **56**, 11196 (2017)

New radiotherapy technology

- Developed gadolinium-loaded nanoparticles that can localize gadolinium at a site close to a tumor cell nucleus
- Destroyed a tumor mass using ten-minute irradiation from monochromatic X-rays
→ Using Auger electrons as an efficient method for destroying tumor mass

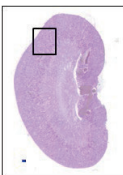


Reference: K. Matsumoto *et al.*, *Sci. Rep.*, **9**, 13275 (2019)

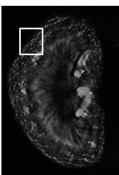
Impacts of diabetes on the glomeruli

- Investigated the impact of diabetes and an antidiabetic drug (SGLT2 inhibitor; SGLT2i) on the numbers and volumes of glomeruli in kidneys
- Explored CT imaging to examine type 2 diabetic *db/db* mice
- Found that diabetes increased glomerular and renal volumes, and SGLT2i increased diabetes-induced renal hypertrophy
→ Improving glucose-lowering effects with SGLT2i for kidneys in diabetic people

Histological image of mouse kidney



X-ray CT image of mouse kidney

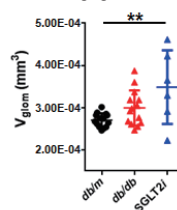


Glomeruli

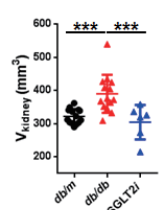
Scale bars, 300 μ m.

Glomeruli can be visualized as bright spots by contrast agent.
Right image: enlarged view in the frame.

Average glomerular volume



Renal volume



Changes in glomerular and renal volumes in spontaneous obesity type 2 diabetic *db/db* mice.

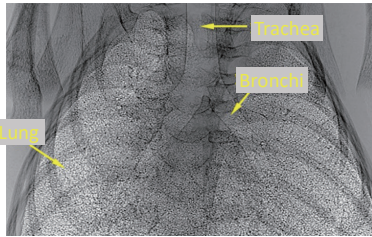


Reference: Y. Takiyama *et al.*, *EBioMedicine*, **36**, 329 (2018)

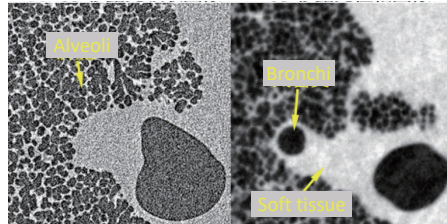
■ Reduction of exposure dose during diagnosis

- Realized high signal-to-noise ratio in CT observations of the chest of a newborn rabbit by capturing the phase shifts of X-rays
- Obtained high quality CT images using a 1/100 exposure dose
→ Reducing the impact of imaging on patient's bodies

X-ray radiograph of the chest of a newborn rabbit.
Fine structure of the alveoli can be recognized.



X-ray CT images of the lung of a newborn rabbit. Left: conventional method with absorption contrast. Right: new method. Adequate image contrast can be obtained in the new method while the exposure dose is 1/100 of that in conventional method.

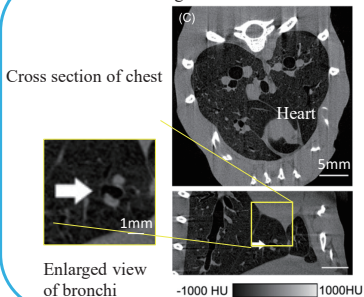


Reference: M. Kitchen *et al.*, *Sci. Rep.*, 7, 15953 (2017)

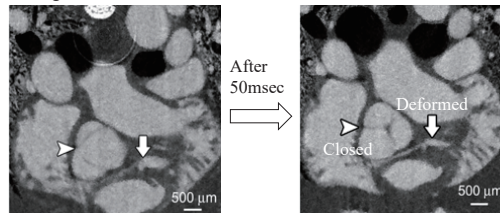
■ Making an accurate diagnosis by capturing slight changes in a body

- Developed an electrocardiographic and respiratory synchronized X-ray micro-CT system for observing the inside of a body
- Visualized the dynamic motion of the cardiovascular system (the coronary arteries and aortic valve)
- Enabling three-dimensional visualization in milliseconds of deformities in the body, minimizing impacts from breathing and heartbeats

CT images of a rat



Deformations in the coronary arteries and aortic valve of a mouse during heartbeat

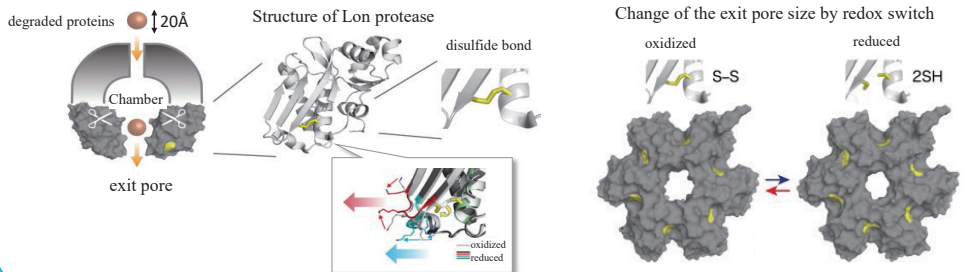


Reference: T. Sera *et al.*, *Phys. Med. Bio.*, 53, 4285 (2008)

Intestinal environment health

- Elucidated the crystal structure of an essential enzyme called Lon for enteric bacteria's existence
 - Discovered a redox switch adapting the enzyme activity between the environments inside the human gut and outside
- Establishing a potential target for infectious diseases caused by these bacteria

BL26B1
BL26B2



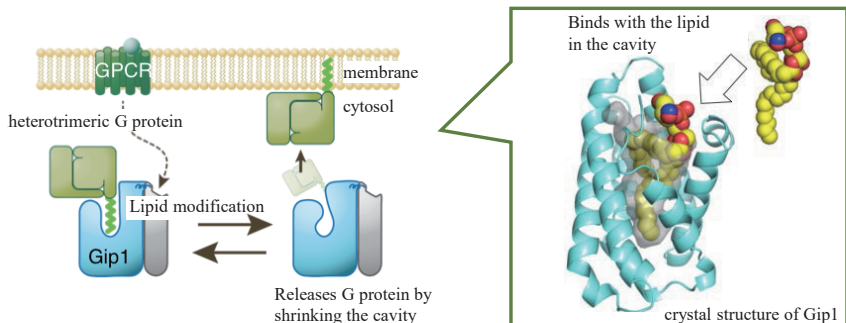
Reference:

W. Nishii *et al.*, *Nature Chemical Biology*, **11**, 46 (2015)

Toward the drug discovery from social amoeba

- Elucidated the crystal structure of Gip1 protein of social amoeba
 - Discovered the Gip1 binding with the lipid modification of heterotrimeric G protein leading to G protein sequestration in the cytosol
- Elucidating the mechanism of G protein-coupled receptor signaling in cells

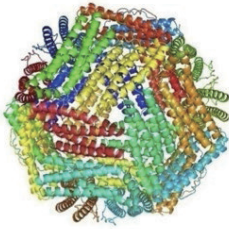
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BL26B2



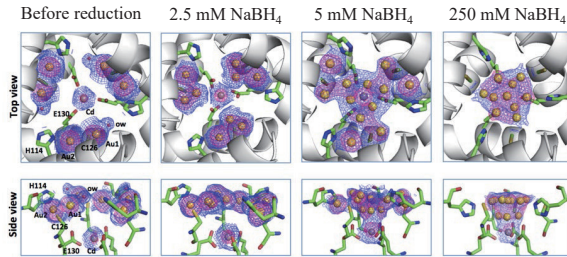
Reference: T. Miyagawa *et al.*, *Nat. Commun.*, **9**, 4635 (2018)

Elucidation of the chemical reactions in protein cages

- Successful crystallization of ferritin in which metal ions move inside the cage
- Observation of gold cluster formation by chemical reduction at atomic resolution
- Elucidating the biomineral formation process



Crystal structure of ferritin



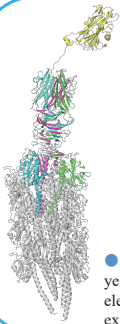
Accumulation of gold ions



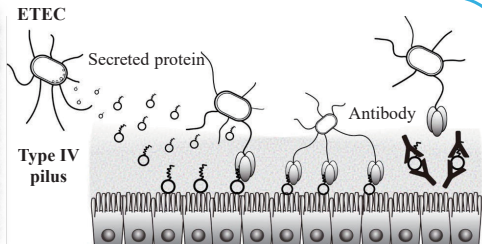
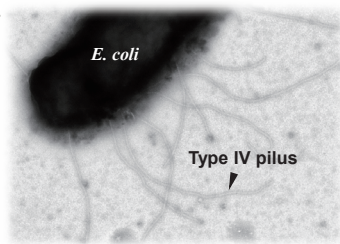
Reference: B. Maity *et al.*, *Nat. Commun.*, **8**, 14820 (2017)

Anti-adhesion therapy to address enteric pathogens

- Elucidated the molecular mechanisms for initial attachment and colonization of enterotoxigenic *Escherichia coli* (ETEC) in the human intestine
- Found the interplay of a secreted protein with type IV pilus to be a crucial step for efficient ETEC colonization of the human intestinal epithelium
- Developing an attractive therapeutic target for anti-adhesive treatment to combat ETEC infections



- Structural model of a secreted protein (colored in yellow) at the tip of type IV pilus (left). Transmission electron microscopy (TEM) image of type IV pili-expressing *E. coli* strain (right).



- Schematic representation of initial attachment of ETEC and its inhibition. A "polyclonal antibody" or "anti-adhesive agent" inhibits the attachment of ETEC by blocking the interaction between secreted protein and type IV pilus.

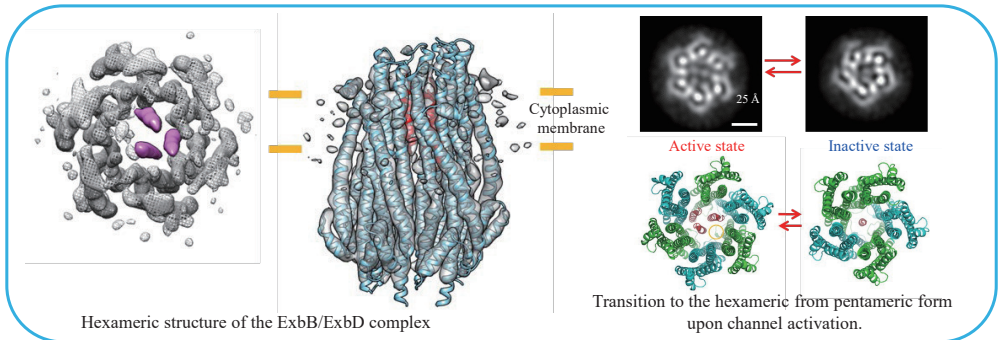


Reference: H. Oki *et al.*, *PNAS*, **115**, 7422 (2018)

Toward drug discovery and fight against bacteria

- Analyzed Structure of an ion channel membrane protein complex ExbB/ExbD by using cryo-electron microscopy and SR X-ray crystallography
 - Revealed a dynamic mechanism of activation/inactivation of the channel associated with morphological changes of the ring-like structure
- Identifying medical applications such as transporting antibiotics and introducing viruses into bacteria

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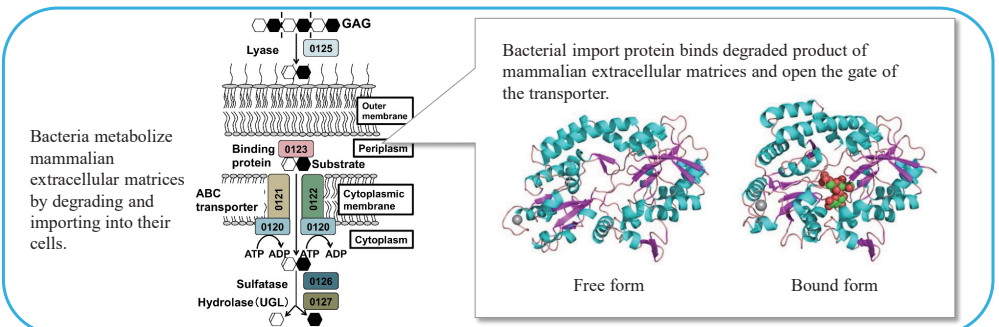


Reference: S. Maki-Yonekura *et al.*, *eLife*, 7, e35419 (2018)

Development of innovative therapy agents for bacterial infections

- Determined the structure of the bacterial import protein complexed with glycosaminoglycan disaccharide, a degradation product of mammalian extracellular matrices
 - Revealed a part of the import system of disaccharide in *Streptobacillus moniliformis*, the causative agent of rat-bite fever
- Enabling molecular design of inhibitors for pathogenic bacterial systems

BL26B1



Reference: S. Oiki *et al.*, *Sci. Rep.*, 7, 1069 (2017)

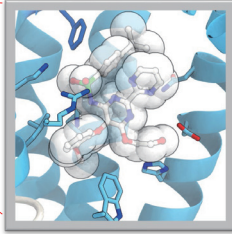
Development of new hypotensive drugs

- Determined the structure of the human endothelin ETB receptor in a complex with hypotensive drug bosentan
- Revealed the inactivation mechanism of the receptor
- Developing drugs based on the microscopic viewpoint

The drug binding mode

Bosentan, a drug for pulmonary arterial hypertension

Zoom-in



How drug works

Drug fits in the pocket
↓
Hormone cannot bind to the receptor
Stop the signaling
↓
Hypotension

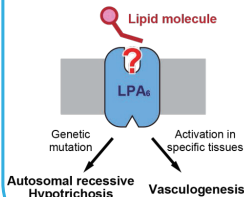


Reference: W. Shihoya *et al.*, *Nat. Struct. Mol. Bio.*, **24**, 758 (2017)

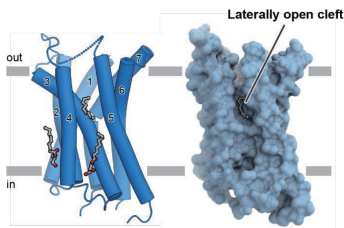
Rational design of therapeutic drugs

- Determined the crystal structure of LPA₆, a membrane receptor involved in autosomal recessive hypotrichosis and angiogenesis in cancer tissues
- Gained insights into ligand recognition and activation mechanism of LPA₆
- Creating a basis for rational design of LPA₆ agonist/antagonist

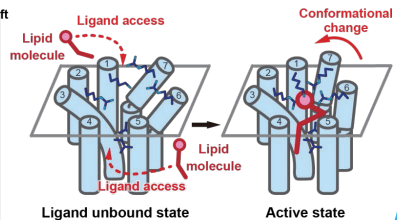
LPA₆ structure remained elusive until recently



LPA₆ structure determined in this study



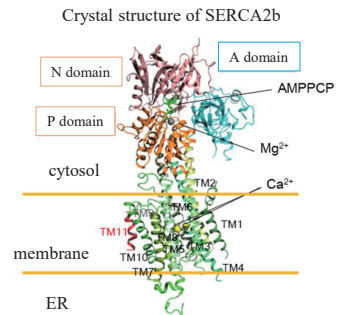
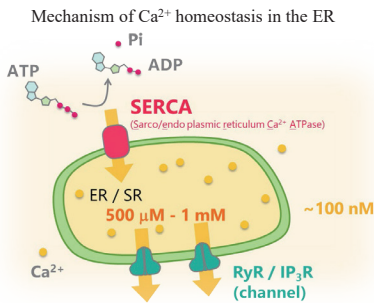
Putative ligand recognition mechanism



Reference: R. Taniguchi *et al.*, *Nature*, **548**, 356 (2017)

■ Elucidation of specific diseases

- Solved the first crystal structure of human ER Ca^{2+} pump SERCA2b
 - Elucidated a mechanism for SERCA2b regulation by its characteristic 11th transmembrane helix TM11
- Providing insights into the molecular mechanisms of Ca^{2+} homeostasis in the ER

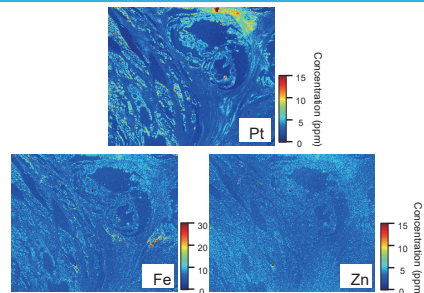
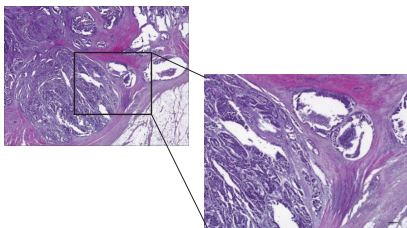


Reference: M. Inoue *et al.*, *Cell Reports*, 27, 1221 (2019)

■ Making chemotherapy safer and more effective

- Visualized platinum distribution in human colorectal cancer tissue after administering an anticancer drug (oxaliplatin)
 - Demonstrated a direct relationship between the distribution of trace elements in tissue and the therapeutic effects of chemotherapy
- Predicting the therapeutic effects of oxaliplatin-based chemotherapy

Representative histopathologic images of rectal cancer sections



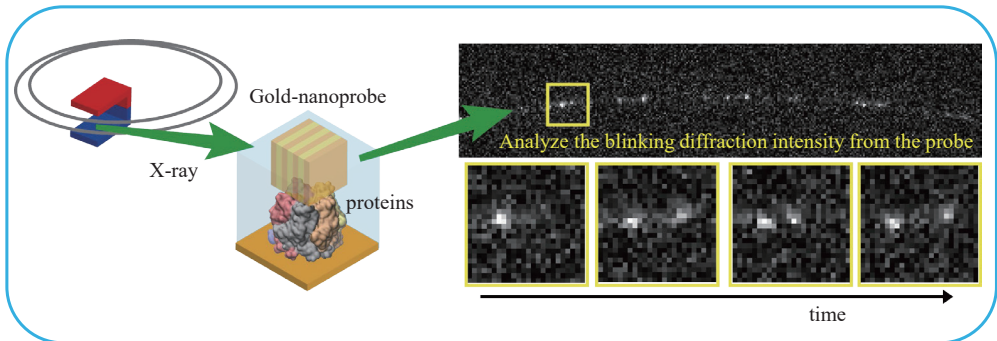
Two-dimensional elemental mapping of platinum (Pt), zinc (Zn), and iron (Fe)



Reference: R. Koba *et al.*, *Int. J. Cancer*, 146(9) 2498 (2020)

Molecular mechanisms of proteins

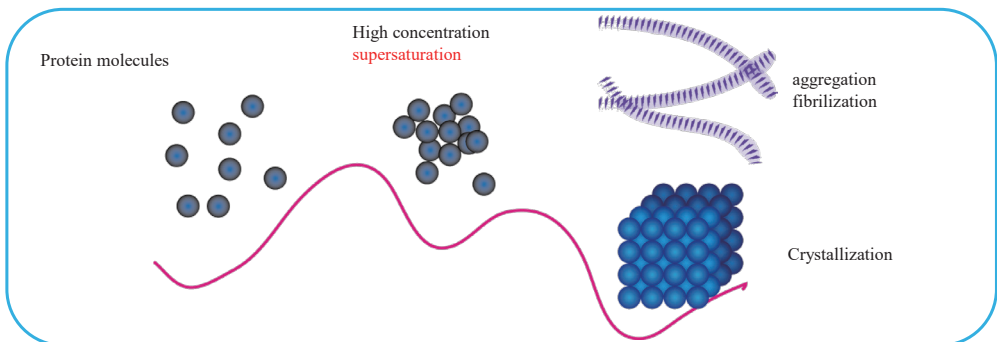
- Tracked the motion of a gold nanoprobe labeled on a single protein with a low X-ray dose
- Analyzing molecular motions in living cells over a long period of time



Reference: Sekiguchi *et al.*, *Sci. Rep.*, **8**, 17090 (2018)

Capture the molecular aggregation process

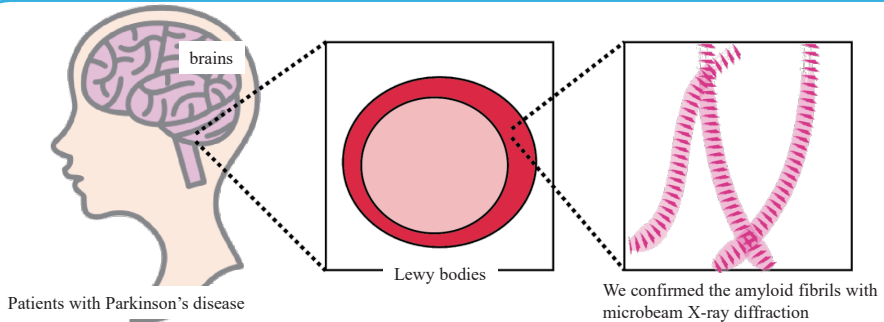
- Investigated a protein that is highly concentrated in the cells, forms a fibril structure and causes neurodegenerative diseases, such as Alzheimer's and Parkinson's diseases
- Captured the aggregation or fibrillization processes for a high concentration of proteins using nanoprobe and X-rays
- Contributing to the development of drugs related to protein concentration and fibrillization



Reference: Y. Matsushita *et al.*, *Sci. Rep.*, **7**, 13883 (2017)

■ Investigating the causes of Parkinson's disease

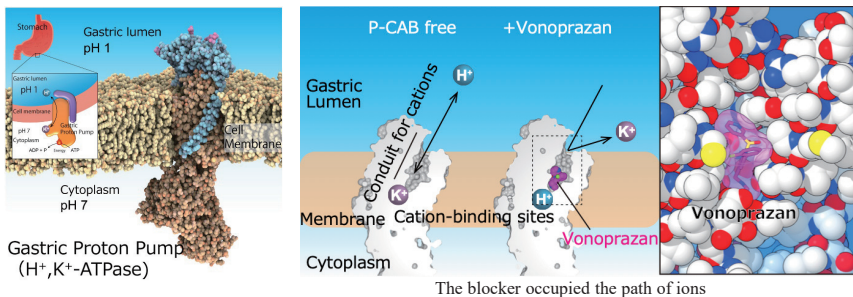
- Detected amyloid fibrils in Lewy bodies within the brains of patients with Parkinson's disease
- Validated propagation experiments using animal and artificial amyloid fibrils
- Contributing to the development of drugs and diagnostic techniques



Reference: K. Araki *et al.*, *Proc. Natl. Acad. Sci. USA*, **116**, 17963 (2019)

■ A healthier stomach environment

- Revealed the mechanisms that cause an acidic environment in stomachs and that repress the secretion of gastric acid using blockers by determining the structures of a gastric proton pump
- Determined the number of transported cations using a gastric proton pump
- Creating guidelines for developing new drugs

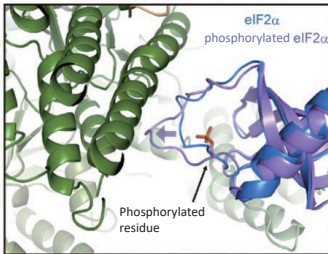


Reference: K. Abe *et al.*, *Nature*, **556**, 214 (2018)
K. Yamamoto *et al.*, *eLife*, **8**:e47701 (2019)

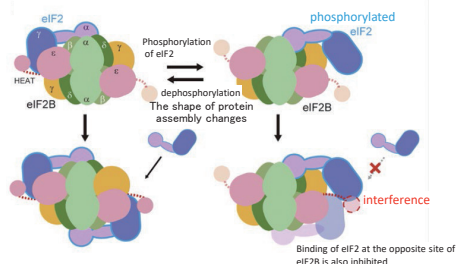
BL32XU
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BL45XU

Discovery of new drugs for neurodegenerative diseases

- Revealed the structure of phosphorylated eukaryotic translation initiation factor 2 (eIF2), which is induced by stress
- Revealed the mechanism by which only one phosphorylation can change the assembly status of proteins and stop protein synthesis
- Understanding the mechanisms of various diseases related to translation initiation factors, such as neurodegenerative diseases



Phosphorylation-induced structure change that was observed in the crystal structure of eIF2B-eIF2α complex



Schematic figure illustrating the control of assembly status by phosphorylation

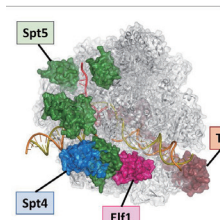


Reference: K. Kashiwagi *et al.*, *Science*, **364**, 6439 (2019)

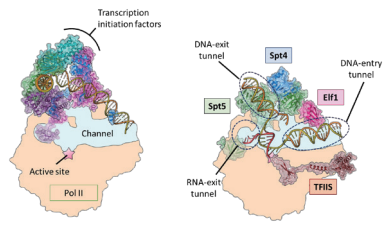
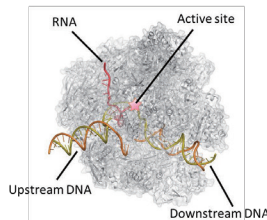
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Mechanisms of transcription and its associated diseases

- Clarified the structure of the elongation complex of RNA polymerase II, which is an enzyme state responsible for mRNA transcription elongation in the eukaryotic nucleus
- Uncovering the detailed mechanisms of transcriptional regulation and diseases caused by its failure



Structure of the complete elongation complex of RNA polymerase II



After elongating a certain length of RNA, the complex undergoes a dramatic change.

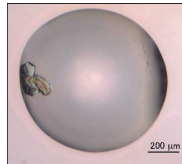
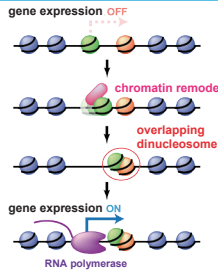


Reference: H. Ehara *et al.*, *Science*, **357**, 921 (2017)

New drugs for cancers

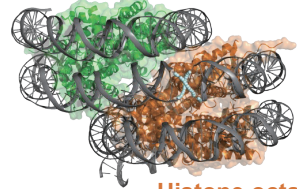
- Revealed the unique crystal structures of overlapping dinucleosomes
- Observing the disability of the nucleosome remodeling that forms overlapping dinucleosomes in certain types of cancer cells

BL32XU
BL41XU
BL45XU



Crystal of the overlapping dinucleosome

Histone hexamer



Histone octamer

Crystal structure of the overlapping dinucleosome

Remodeling of nucleosomes induces the overlapping dinucleosome formation and may induce gene expression.



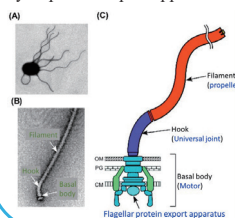
Reference: D. Kato *et al.*, *Science*, **356**, 205 (2017)

Development of new types of drugs to fight infectious disease

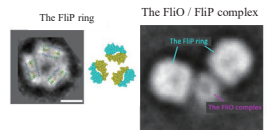
- Determined the structure of FliP, a core component of the flagellar protein export apparatus
- Revealed the assembly mechanism of the export gate complex
- Developing new anti-infective drugs that target the export gate complex

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BL41XU
BL45XU

Bacteria move using the flagellum. The flagellum is constructed by the component proteins exported by a specific export apparatus.

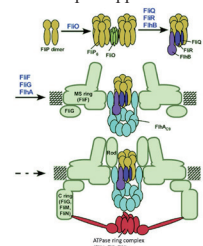


The flagellar protein export apparatus is composed of a gate complex and an ATPase complex



Structures of an export gate protein, FliP, and its assembly scaffold, FliO, in complex with FliP were studied by X-ray crystallography and Cryo electron microscopy. Three dimeric units of FliP form a ring with 10 nm diameter.

The construction pathway of the export apparatus.

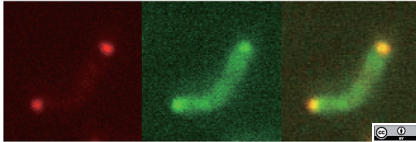


Reference: T. Fukumura *et al.*, *PLoS Biol.*, **15**, e2002281 (2017)

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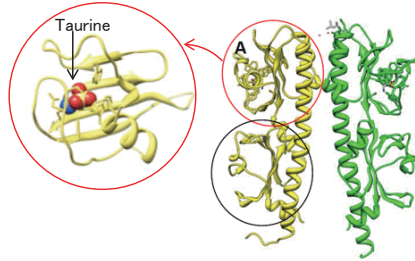
■ Eradication of bacterial infectious diseases

- Discovered that taurine, a component of human bile, attracts *Vibrio cholerae*
- Revealed the mechanism of taurine sensing by the structure of Mlp37, a sensor protein of *V. cholerae*
- Developing new types of drugs that control the behavior and toxin production of *V. cholerae*



Location of Mlp37 in *V. cholerae* Location of serine in *V. cholerae* Superposition of the left two panels

Mlp37 is a sensor protein that detects taurine and various amino acids, such as serine. Mlp37 is localized at the bacterial cell poles.



Structure of Mlp37 in complex with taurine

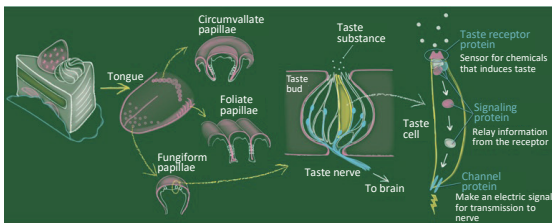


Reference: S. Nishiyama *et al.*, *Sci. Rep.*, **6**, 20866 (2016)

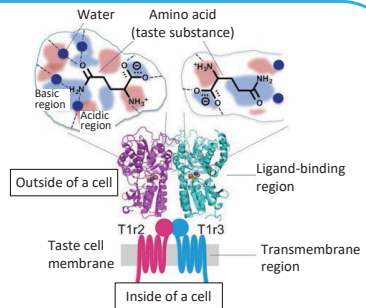
BL32XU
BL41XU
BL45XU

■ Understanding how we can sense taste

- Determined the structure of the sensor region of a taste receptor, T1r2-T1r3
- Revealed the mechanism for recognizing amino acids, a taste substance
- Understanding how we recognize specific tastes, leading to the development of new taste substances



Process of taste sensation



Structure of taste receptor T1r2-T1r3

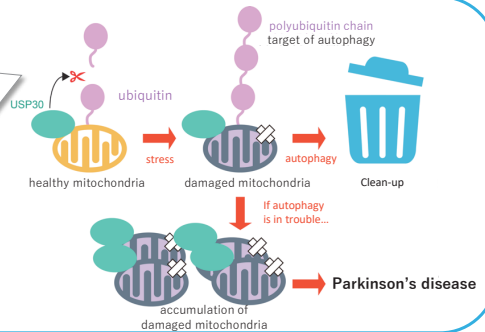
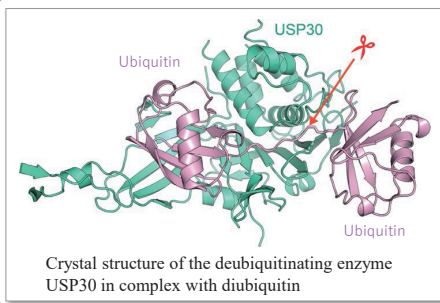


Reference: N. Nuemket *et al.*, *Nat. Commun.*, **8**, 15530 (2017)

Development of medications for Parkinson's disease

- Determined the crystal structure of UPS30, an enzyme which cleaves poly-ubiquitin chains on damaged mitochondria
 - Found the binding manner of UPS30 on poly-ubiquitin chains to cleave to be different from other de-ubiquitination enzymes
- Providing information for developing compounds that inhibit specific enzymes

BL32XU
BL41XU
BL45XU

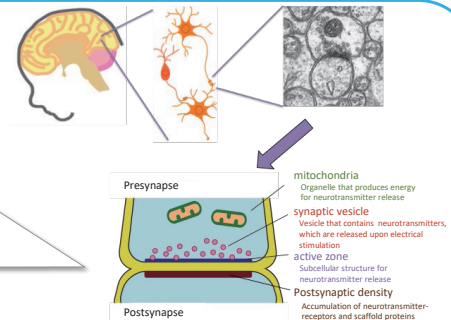
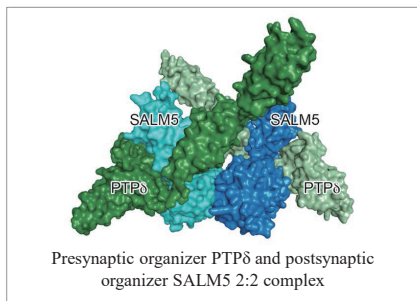


Reference: Y. Sato *et al.*, *Nat. Struct. Mo. Bio.*, **24**, 911 (2017)

Understanding the cause of neuro-developmental disorders

- Determined the crystal structure of the 2:2 complex of presynaptic organizer PTPδ and postsynaptic organizer SALM
 - Revealed that the 2:2 binding manner is important for binding specificity and correct trans-synaptic adhesions
- Understanding a structural basis for controlling specificity in synapse synthesis in the central nervous system

BL32XU
BL41XU
BL45XU

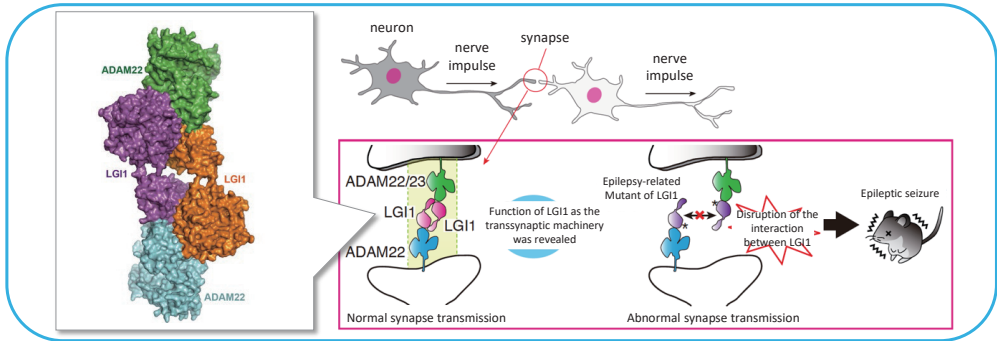


Reference: S. Goto-Ito *et al.*, *Nat. Commun.*, **9**, 269 (2018)

BL38B1
BL41XU

Molecular mechanisms in synaptic transmission in epileptic disorders

- Determined the crystal structure of the causative protein of epilepsy LGI1, complexed with its receptor ADAM22
- Revealed the machinery for precise synaptic transmission by the LGI1-ADAM22 trans-synaptic complex
- Detecting LGI1 mutations to understand the causes of epilepsy

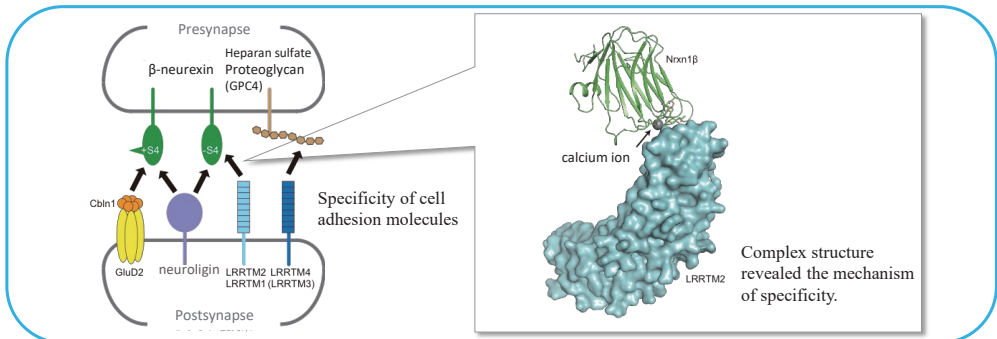


Reference: A. Yamagata *et al.*, *Nat. Commun.*, **9**, 1546 (2018)

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BL41XU
BL45XU

Research on neuro-developmental disorders

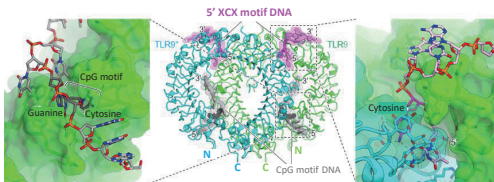
- Determined the crystal structure of cell adhesion factor LRRTM2 complexed with Nrnx1β via Ca^{2+} ions
- Revealed the molecular mechanisms of binding specificity to connect synaptic cells properly
- Understanding specificity in synapse synthesis in the central nervous system



Reference: A. Yamagata *et al.*, *Nat. Commun.*, **9**, 3964 (2018)

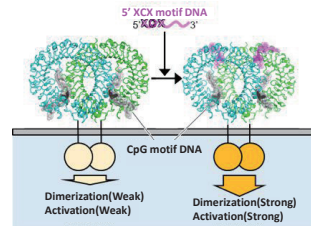
Development of antiviral drugs and vaccines

- Investigation of how the toll-like receptor 9 (TLR9) senses the DNA sequence of a microorganism entering the body and triggers an innate immune response
 - Elucidation of a detailed activation mechanism for TLR9
- Developing new drugs that target TLR9



"DNA with known CpG motif sequence" + "DNA with second cytosine from terminal" are important for TLR9 activation and bind to different sites.

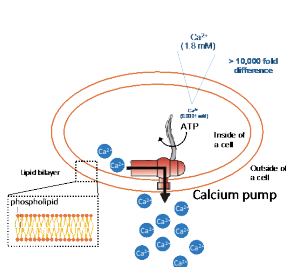
TLR9 is activated by forming a dimer. TLR9 and the two DNAs efficiently bound in a ratio of 2: 2: 2.



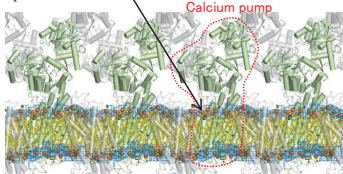
Reference: U, Ohto *et al.*, *Immunity*, **48**, 649 (2018)

Development of new drugs targeting specific membrane proteins

- Determined the structure of a calcium pump that controls muscle contractions together with phospholipids
 - Demonstrated the important roles of the phospholipids that surround membrane proteins in achieving the biological functions of the membrane proteins
- Understanding the mechanisms of membrane proteins that constitute the majority of pharmaceutical targets

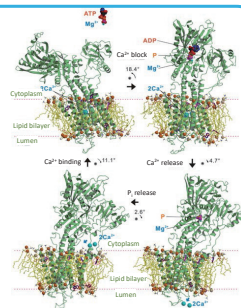


Visualization of phospholipids that surround a pump protein



Structure of the calcium pump crystal

Phospholipids are incorporated into the mechanism for pumping calcium ions



Reference: Y. Norimatsu *et al.*, *Nature*, **545**, 193 (2017)

Clarifying the mechanisms related to the onset of Parkinson's disease

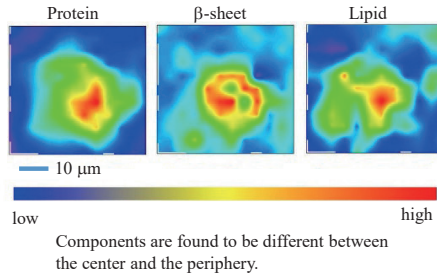
- Analyzed the structure of the Lewy bodies in the brains of Parkinson's disease patients
- Developing a new method for Parkinson's disease treatment

Parkinson's disease

The disease are developed by the cell death of neurons in the substantia nigra of the brain. Tremors, stiffness or slowing of movement are commonly caused.

Lewy bodies

Lewy bodies are formed by abnormal changes in the proteins that make up neurons in the substantia nigra of the brain. They are said to be deeply involved in the development of Parkinson's disease.

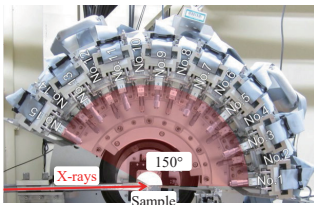


Reference: K. Araki *et al.*, *Sci. Rep.*, **5**, 17625 (2015)

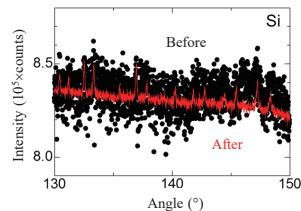
Diagnostics by imaging

- Development of "ReLiEf", visualizing signal underneath the noise in X-ray detectors
- Improving the quality of X-ray data

X-ray detector system for structural analysis



Before and after the correction of X-ray data



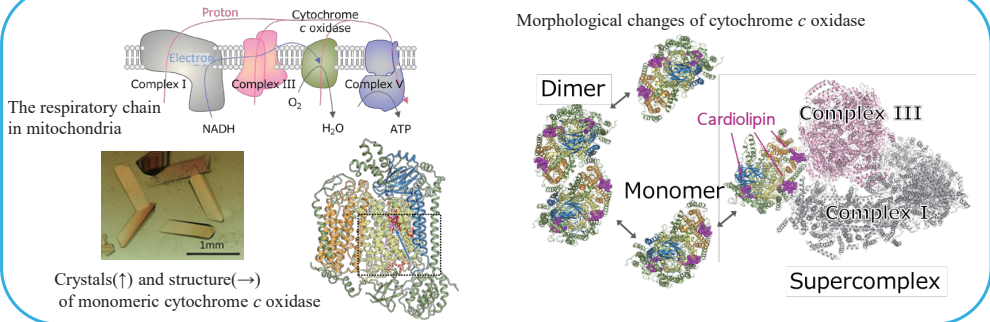
Visualizing signal underneath noise



Reference: K. Kato *et al.*, *J. Synchrotron Rad.*, **26**, 762 (2019)

Energy production mechanisms in the human body

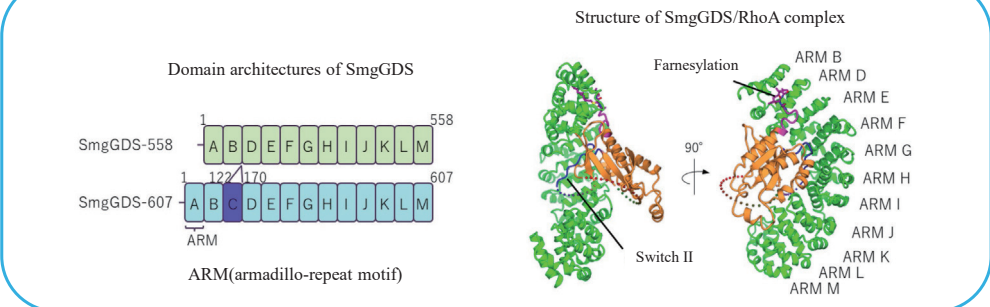
- Solved the structure of cytochrome *c* oxidase, a terminal oxidase in the respiratory chain, in a different assembly state
 - Found the enzymatic activity to be different depending on the assembly states
- Understanding how to regulate activity by changing the morphology



Reference: K. Shinzawa-Itoh *et al.*, *PNAS*, **116**, 19945 (2019)

Development of new anticancer drugs

- Solved the structure of a small GTP-binding protein (RhoA) and its regulator (SmgGDS-558) complex
 - Revealed the RhoA recognition mechanism of SmgGDS-558
- Elucidating the mechanisms of cytoskeleton formation and cell proliferation



Reference: H. Shimizu *et al.*, *PNAS*, **115**, 9563 (2018)

Critical clues for discovering new pharmaceutical drugs

- Solved a longstanding mystery regarding the mechanisms of blood degradation at the atomic scale
- Visualized the production mechanisms of bilirubin, a cause of jaundice
→ Contributing to the development of new pharmaceuticals

Degradation steps of red blood cells



A bruise: we can see the blood degradation process through the skin.



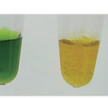
Jaundice



Blood components (heme)

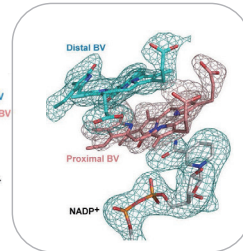
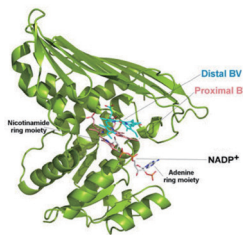


Reaction intermediates (biliverdin)



Cause of jaundice (bilirubin)

Visualization of production mechanism of bilirubin



Mechanism in which the substrate itself works as a catalyst is extremely unique.



Reference: H. Takao *et al.*, *Nat. Commun.*, **8**, 14397 (2017)

Understanding the sources of dysfunction in molecular motors

- Solved the atomic structure of the motor protein (dynein), which transports various cargo within cells
- Revealed the moving mechanism on a walking track (microtubule) in the cell using a long leg-like structure
→ Understanding the molecular motors that drive the ciliary flagellar beating of fallopian tubes or sperm cells

ATP-binding ring (Head)



Crystal structure of dynein

Track-binding domain (Leg)

Mechano-chemical coupling (Arm)

Microtubule (intracellular track)

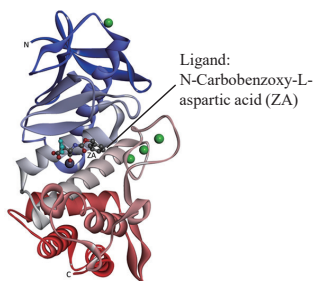


Reference: T. Kon *et al.*, *Nat. Struct. Mol. Biol.*, **18**, 638 (2011)
T. Kon *et al.*, *Nature*, **484**, 345 (2012)

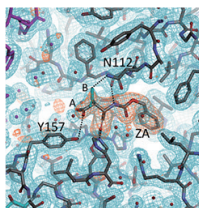
Application of XFEL for drug discovery

- Room-temperature structure analysis of protein-ligand complexes, close to physiological conditions
- Contributing to structure-based drug design

Structure of thermolysin-ligand complex

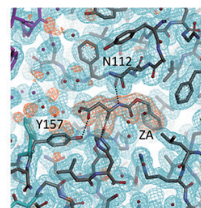


Structures observed under room-temperature and cryogenic conditions.



Room temperature (XFEL)

Clear difference in this part of the ligand



Cryogenic condition
(synchrotron radiation)



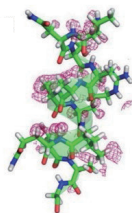
Reference: H. Naitow *et al.*, *Acta Cryst. D*73, 702 (2017)

Understanding the structure-function relationships of enzymes

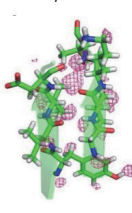
- Analyzed the precise structures of proteinase K at room temperature
- Determined interatomic distances in proteins at a resolution of 1.2 Å
- Contributing to the development of drugs and functional molecules

Partial structures of proteinase K

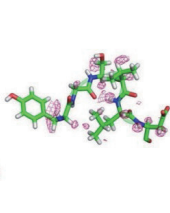
Helix



β-strand

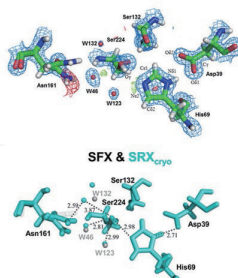


Turn structure



Hydrogen atoms are distinguishable
(marked in red).

Structure around the active site



Water molecules (W46, W123, W132) are clearly distinguished.

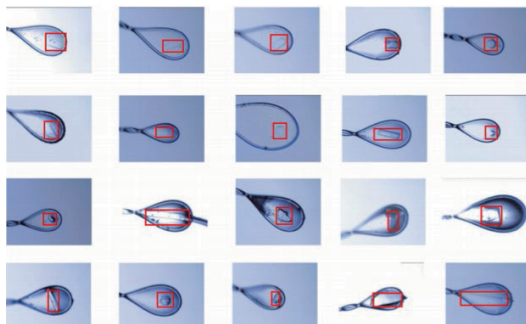
Clear difference between the room-temperature (gray) and cryogenic (cyan) structures



Reference: T. Masuda *et al.*, *Sci. Rep.*, 7, 45604 (2017)

Automatic crystal detection program

- Developed “DeepCentering,” a program to detect a protein crystal based on image processing using a deep learning algorithm
- Implemented the program at a beamline to automate crystal centering
- Developing important steps to achieve fully automatic protein crystallography



Frozen protein crystals in the cryo-loop mounted on the beamline equipment for diffraction data collection. Red squares are the result of automatic detection.



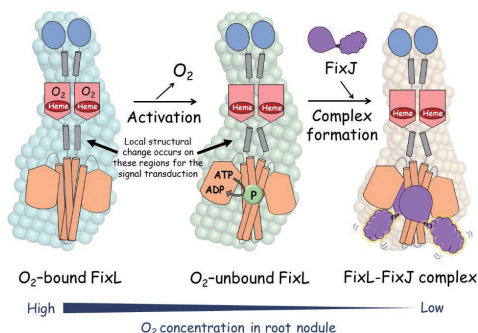
Reference: S. Ito *et al.*, *J. Synchrotron Rad.*, **26**, 1361 (2019)

Fundamental Biology

Architecture of proteins involved in nitrogen fixation in symbiotic plants

- Elucidated the whole structure of the FixL/FixJ protein complex of a symbiotic nitrogen-fixing bacterium in the root nodules of soybeans
- Discovered the signal transduction system involved in sensing environmental changes in low-oxygen conditions
- Developing symbiotic strains that can be effective in barren soil environments

BL26B2
BL38B1
(former BL45XU)



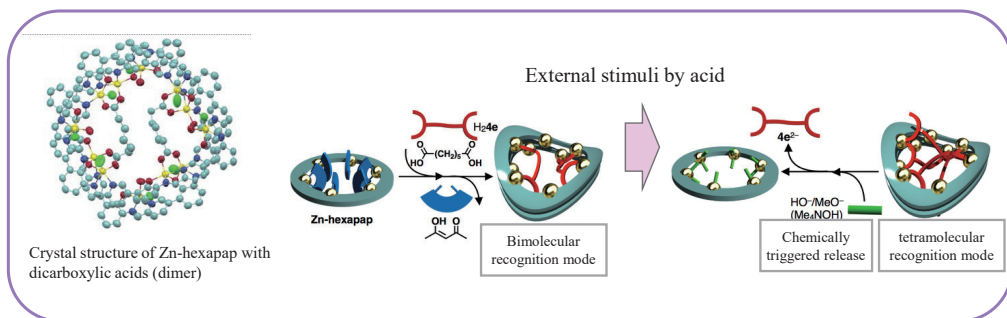
Signal relay mechanism under low-oxygen conditions accompanied with the phosphotransfer from FixL to FixJ.



Reference: S. A. Gareth *et al.*, *Science Signaling.*, **11**, eaaq0825 (2018)

Platform for innovative allosteric catalysts and selective molecule sensors

- Developed a multinuclear zinc complex synthesized from a macrocyclic ligand, hexapap, with inwardly arranged labile metal coordination sites for external molecules
 - Found that external stimuli with acid/base utilization controls the binding mode of guest dicarboxylic molecules
- Enabling the binding and controlling of small molecules via multiple coordination bonds

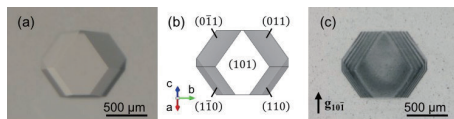


Reference: T. Nakamura *et al.*, *Nature Comm.*, **8**, 129 (2017)

High accuracy structural analysis of protein crystallography

- Observed dynamical diffraction, which occurs in high-quality crystals such as silicon, in a protein crystal for the first time
- Meeting the need for a dynamical diffraction model in crystallography and model refinement

The crystals in the X-ray topograph are clearly observed fringe contrasts similar to Pendellösung fringes exhibiting a high crystal quality.



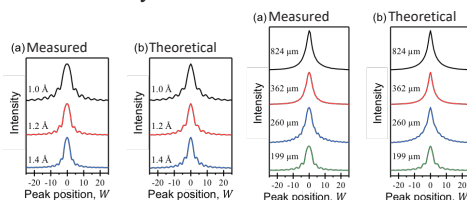
GI crystal viewed

(a) Optical micrograph

(b) Corresponding schematic

(c) X-ray topograph

From the rocking curve of protein crystal observed dynamical diffraction at first time.



The period of oscillation of the rocking curve profile change with X-ray wavelength.

The period of oscillation of the rocking curve profile change with crystal thickness.

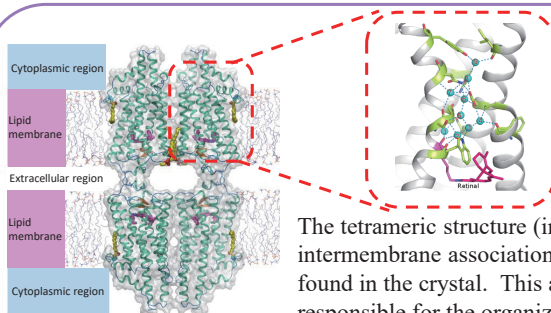


Reference: R. Suzuki *et al.*, *Proc. Natl. Acad. Sci. USA*, **115** (14), 3634 (2018)

BL26B1
BL26B2
BL32XU
BL41XU
BL45XU

Intracellular and extracellular signaling molecular switches

- Revealed the tetrameric structure of the squid light sensor protein rhodopsin
- Found that the membrane protein expresses its function when embedded in the cell membrane
- Developing detailed models of many G-protein-coupled receptors (GPCRs)



Invertebrate phototransduction uses an inositol-trisphosphate signalling cascade, in which photoactivated rhodopsin stimulates a G_q -type G protein.



100um

Squid rhodopsin crystal

The tetrameric structure (intramembrane plus intermembrane association) of rhodopsin was found in the crystal. This assembly may be responsible for the organization of microvillar membranes in the photoreceptor rhabdom.



Reference: M. Murakami & T. Kouyama, *Nature*, **453**, 363 (2008)

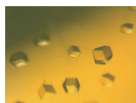
Fundamental Biology

BL26B1
BL26B2
BL41XU

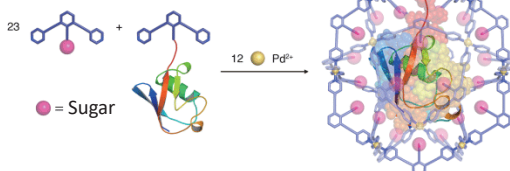
Protein encapsulation within synthetic molecular hosts

- Found the encapsulation of a small protein, ubiquitin, within giant coordination cages
- Discovering various applications in industrial and drug discovery fields, such as protein structure analysis and function modification

Protein encapsulation was achieved via coordination self-assembly of protein- or sugar-attached organic ligands and $Pd(II)$ ions to form the nanocage with a diameter of 7 nm surrounding the targeted protein.



Artificial protein-encapsulated crystals



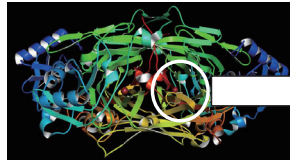
Reference: D. Fujita *et al.*, *Nat. Commun.*, **3**, 1093 (2012)

In crystallo protein thermodynamic analysis

- Elucidated the structural change mechanisms of enzyme proteins in non-frozen crystals under controlled temperature and humidity
- Determined the thermodynamic parameters of the conformational changes by collecting X-ray diffraction data at different temperatures
- Providing physicochemical analysis based on the structures and functions of “the active states”

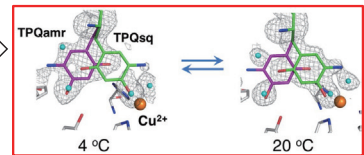


Crystal of a copper amine oxidase from *Arthrobacter globiformis* (AGAO)



Structure of AGAO
(PDB:1IVU)

Equilibrium state is affected by temperature



These experiments were performed using the Humid air and glue-coating (HAG) method.

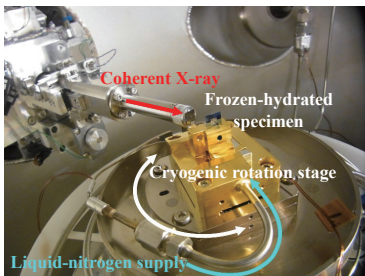


Reference: T. Murakawa *et al.*, *PNAS*, **116**, 135 (2019)

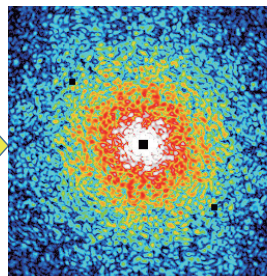
Whole cell visualization with negligible radiation damage

- Analyzed the three-dimensional structures of frozen-hydrated cell specimens and non-crystalline specimens
- Enabling innovative microscopy complementary to visible fluorescence microscopy and transmission electron microscopy

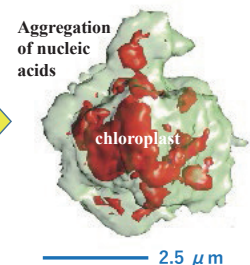
Apparatus for cryogenic tomography experiment



Diffraction pattern from a cell



Three-dimensional reconstruction with resolution higher than 50 nm

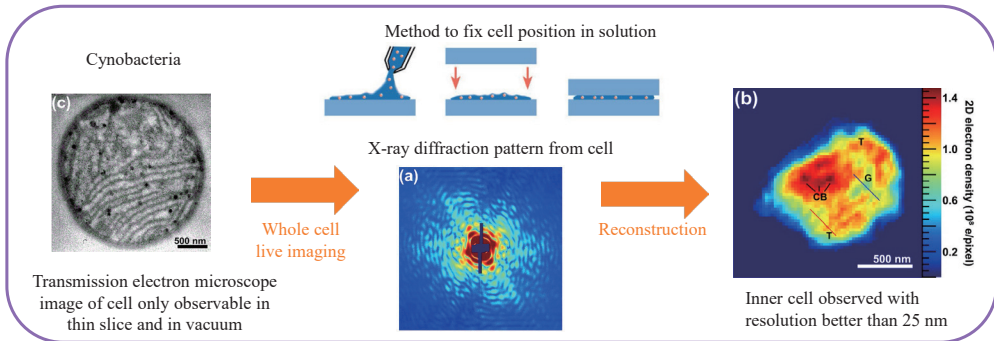


Reference:

A. Kobayashi *et al.*, *J. Synchrotron Rad.*, **25**, 1803 (2018)

Interior imaging of a living cell in a solution

- Visualized inner cell structures in solution with a resolution greater than 25 nm
- Observing the interiors of living cells (currently not feasible using an electron microscope)

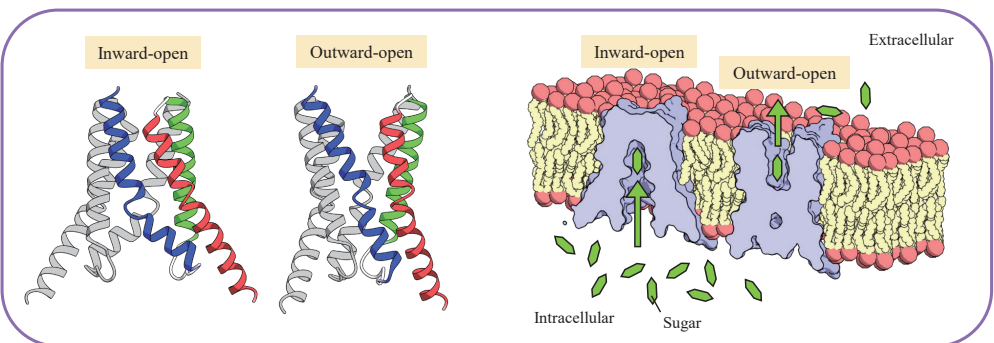


Reference:

D. Nam *et al.*, *Phys. Rev. Lett.*, **110**, 098103 (2013)

Determining how cells can transport nutrients across cell membranes

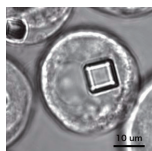
- Determined the crystal structure of SWEET, a sugar transport protein discovered in 2010
- Revealed that the mechanism by which sugar molecules pass through membranes is the motion of their hinge region when two SWEETs assemble with each other
- Understanding more clearly the nutrient transport mechanism, enabling greater crop yields



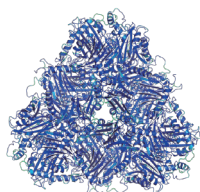
Reference: Lee *et al.*, *Nat. Commun.*, **6**, 6112 (2016)

Intracellular molecular accumulation

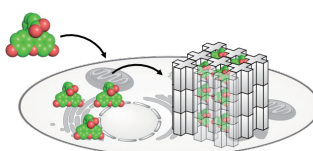
- Creation of a molecular sieve using *in vivo* protein crystals, which form porous crystalline materials by deleting the amino acid residues of polyhedra crystals
 - Selective accumulation of target molecules in living cells
- Enabling *in vivo* crystal structure analysis of cellular molecules



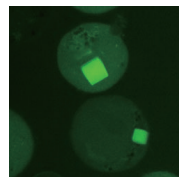
Insect cells produced polyhedra crystal



Assembly structure of polyhedra mutant crystal



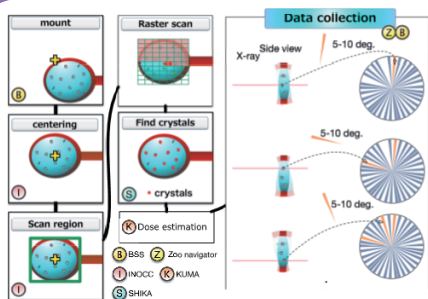
Adsorption of fluorescent dyes into the polyhedra mutant crystal in insect cells



Reference: S. Abe *et al.*, *ACS Nano*, **11**, 2410 (2017)

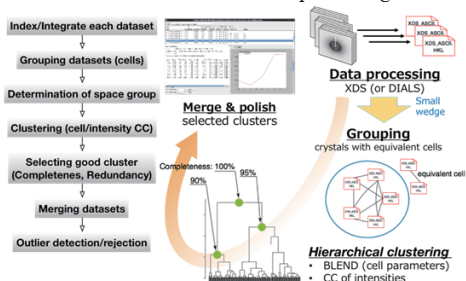
More efficient data processing for protein crystallography

- Developed an automatic data processing/merging program to perform structural analyses on tiny and/or weakly-diffracting protein crystals
- Merging many datasets into high resolution data and performing nearly fully automated data merging, polishing, and result browsing



> Data processing with KAMO

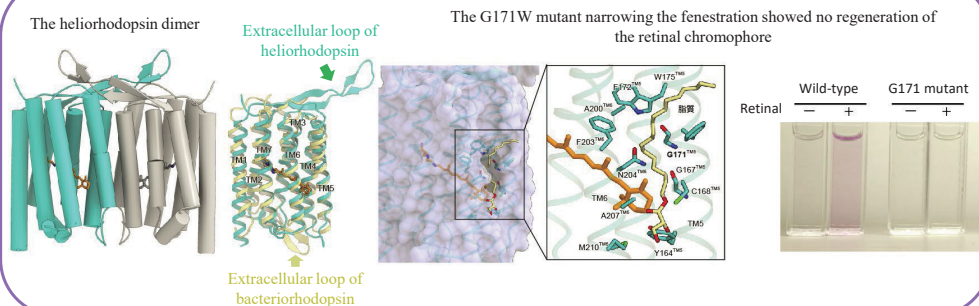
Flow of KAMO data processing



Reference: K. Yamashita *et al.*, *Acta Cryst.* D74, 441 (2018)

Structure of heliorhodopsin, a new photosensitive protein

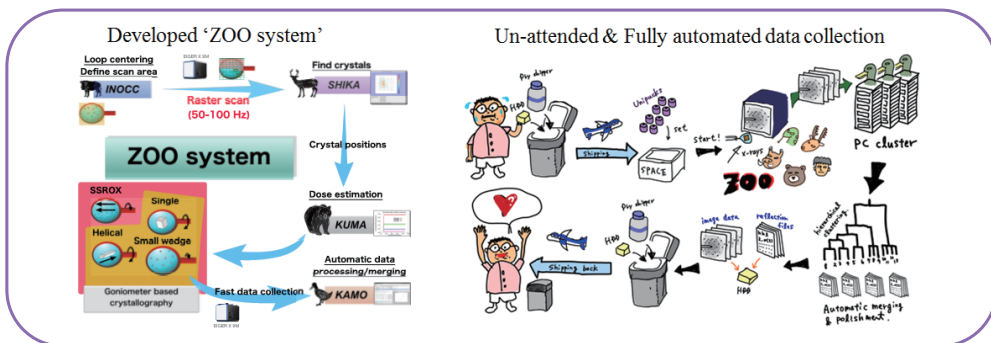
- Investigating heliorhodopsin, which shares a common fold with bacteriorhodopsin and is embedded in membranes in inverted orientations
- Identifying lateral fenestration to be a key to capturing the retinal chromophore
→ Uncovering the similarity and diversity among microbial rhodopsins



Reference: W. Shihoya *et al.*, *Nature*, **574**, 132 (2019)

Unattended and automated data collection for protein crystallography (MX)

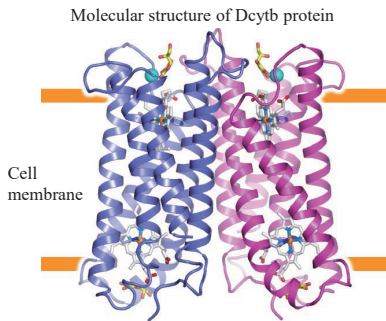
- Developed a fully automated data collection system for MX
- Enabled non-experts to obtain high resolution data
→ Enabling a wider range of users and fields to use MX for their research



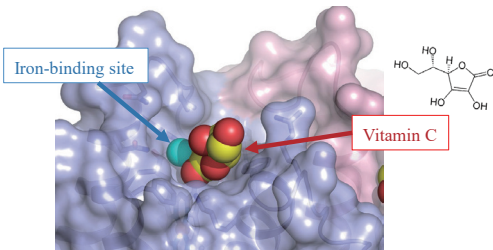
Reference: K. Hirata, K. Yamashita *et al.*, *Acta Cryst.* D75, 138 (2019)

Vitamin C and the absorption of dietary iron

- Structural analysis of human Dcytb protein revealed the mechanism of electron transfer from vitamin C to Fe^{3+} , an essential process for iron transport
- Developing new strategies for promoting the absorption of dietary iron



Dcytb creates a space on its molecular surface to bind vitamin C to transfer electron to Fe^{3+}



Reference: M. Ganasen *et al.*, *Commun. Biol.*, **1**, 120 (2008)

Using new nanoparticles to deliver drugs to affected areas

- Studied the structure of new nanoparticles that can deliver drugs to affected areas
- Found the drug at the core of the nanoparticle soaked into the shell of the particle
- Developing nanoparticles that can efficiently deliver drugs to only relevant areas

The nanoparticles play a role in delivering drugs to affected areas.



Nanometer scale

We investigate the distribution of the drugs inside the nanoparticle. This knowledge is related to delivering the drugs to the affected area.

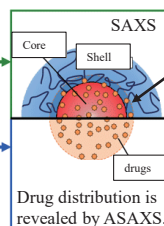
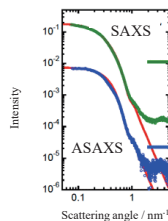
Methods

ASAXS measurement

Incident X-ray



Measure the distribution of drugs



The drugs were soaked here!

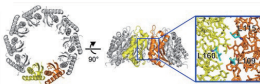


Reference: Y. Sanada *et al.*, *J. Am. Chem. Soc.*, **135** 2574 (2013)

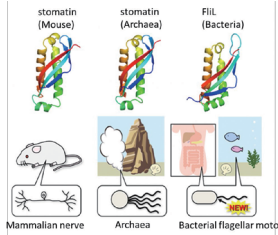
Power control of the bacterial flagellar motor

- Investigated the enhancement process of the output of the bacterial flagellar motor by FliL, depending on its environmental load
 - Revealed that the structures of FliL resembles those of mammalian stomatin proteins in nerves and erythrocytes, implying that FliL and the stomatin proteins share a common functional mechanism
- Understanding and designing biological motors at a nano-scale

The structure of FliL_C

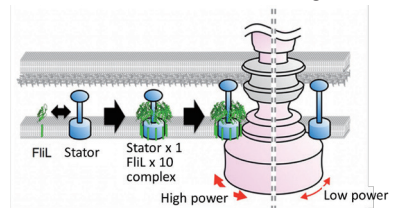


FliL forms a ring composed of 10 FliL molecules.



FliL shares a common structure with the mammalian stomatin family proteins.

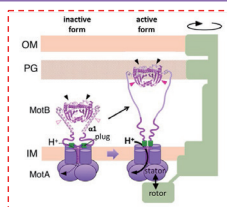
FliL forms a complex around the stator. The stator is activated by the interaction with the inner surface of the FliL ring.



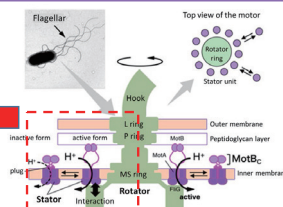
Reference: N. Takekawa *et al.*, *mBio*. **10** (2), e00292 (2019)

Activation mechanisms of the bacterial flagellar motor

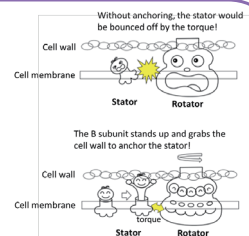
- The flagellar motor consists of the rotor and the stator, and the stator is activated only when incorporated into and anchored around the rotor.
 - X-ray crystallography and NMR analysis revealed the mechanisms for stator activation and anchoring.
- Understanding biological motors, enabling the development of new types of drugs to fight infections



The structural change of MotB, a stator subunit protein, couples the opening of the ion channel with anchoring of the stator to the bacterial cell wall.



The ion flow through the channel in the stator induces the interaction between the stator and the rotor for torque generation.



The stator should be anchored somewhere, otherwise it would be bounced off by the torque.

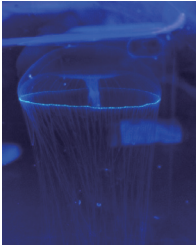


Reference: S. Kojima *et al.*, *Structure*, **26**, 590 (2018)

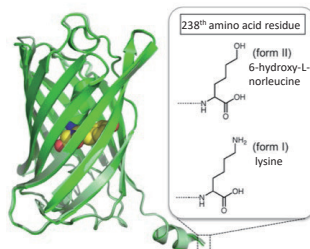
BL32XU
BL41XU
BL45XU

New tools for life sciences

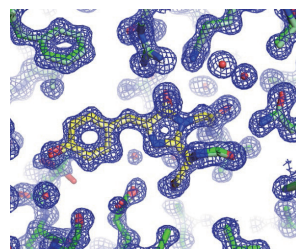
- Determined the structure of the green fluorescent protein (GFP) that locates in the photogenic organ of jellyfish and is responsible for light emission
 - Revealed the structures of two slightly different GFPs expressed in *Escherichia coli*
- Providing basic information about the development of “fluorescent labeling” tools



Jellyfish, *Aequorea Victoria*. The position that emits green light is a photogenic organ (Kyoto Aquarium)



Structure of green fluorescent protein (GFP)



Structure around chromophore of GFP

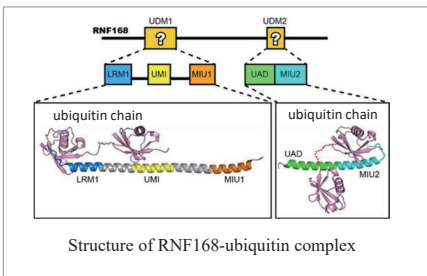


Reference: T. Nakatani *et al.*, *Sci. Rep.*, **9**, 4722 (2019)

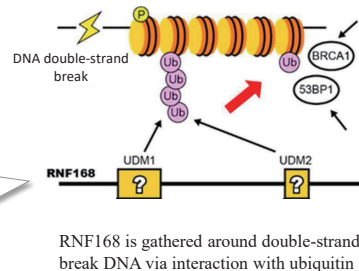
BL32XU
BL41XU
BL45XU

Suppressing carcinogenesis and radiation competency

- Determined the crystal structure of E3 ubiquitin ligase RNF168
 - Revealed the mechanism for gathering RNF168 around double-strand break DNA via interactions with ubiquitin
- Contributing to the prevention of cancerous growths through understanding the process required for recovery from double-strand breaks



Structure of RNF168-ubiquitin complex



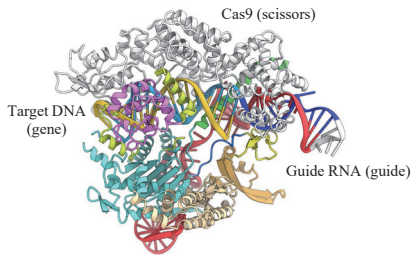
RNF168 is gathered around double-strand break DNA via interaction with ubiquitin



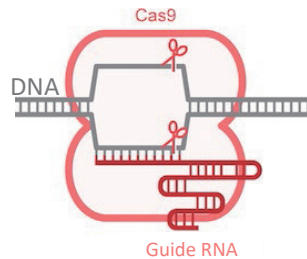
Reference: T. S. Takahashi *et al.*, *Nat. Commun.*, **9**, 170 (2018)

■ Development of new genome-editing technologies

- Determined the crystal structure of the Cas9-guide RNA-target DNA complex
- Revealed the DNA cleavage mechanism for the Cas9-guide RNA complex
- Developing more efficient genome-editing technologies



The Cas9-guide RNA-target DNA complex structure



DNA cleavage mechanisms by the Cas9-guide RNA complex

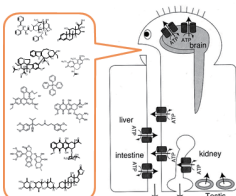
Reference: Nishimasu *et al.*, *Cell*, **156**, 935 (2014)

Fundamental Biology

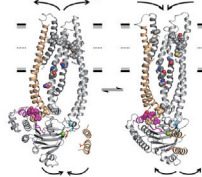
■ Methods for transporting various drugs

- Determined two structure types (inward facing and outward facing states) of P-glycoprotein (ABCB1), which carries drugs out of cells
- Revealed the participation of these structural elements in the mechanism that transports various drugs out of cells
- Developing new innovative drugs

How does P-glycoprotein pump various drugs in one direction?



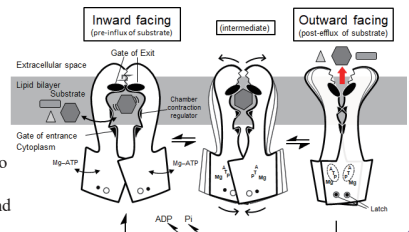
Inward facing Outward facing



ABCB1 structures of two states

- Inward facing state open inside cell to capture the drug
- Outward facing state bind the ATP and carry the drug out of the cell

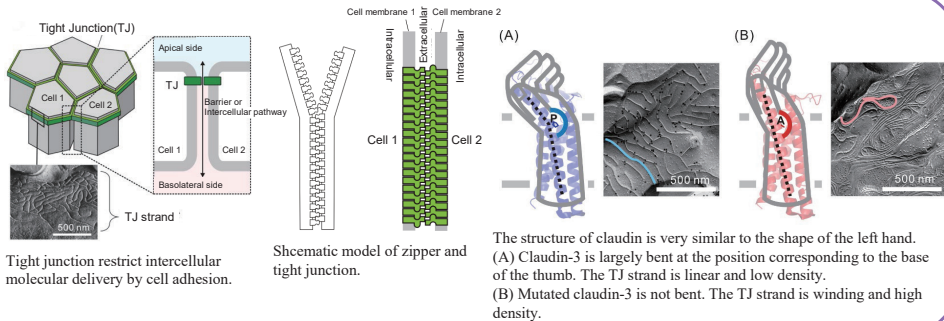
Capture various drugs in a huge inner bag and pump out.

Reference: A, Kodan *et al.*, *Nat. Commun.*, **10**, 88, (2019)

BL32XU
BL41XU
BL45XU

New intercellular methods for drug delivery

- Analyzed the crystal structures of Claudin-3, the component of a tight junction that forms a barrier and/or a channel in cellular spaces by cell adhesion
 - Revealed the difference of one residue in the transmembrane domain of claudin, affecting the morphology and adhesiveness of the tight junction
- Developing applications for new intercellular methods for drug delivery

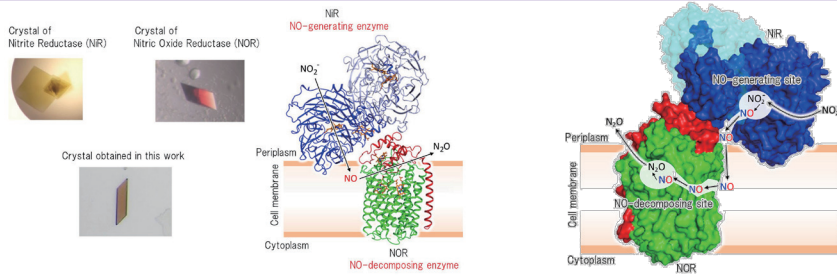


Reference: S. Nakamura *et al.*, *Nat. Commun.*, **10**, 816 (2019)

BL32XU
BL41XU
BL45XU

Mechanisms for various physiological responses

- Revealed the quick decomposition of cytotoxic NO by the complex of nitric oxide (NO)-generating nitrite reductase (NiR) and NO-decomposing membrane-integrated NO reductase (NOR)
- Applying the reaction system based on denitrification to other physiological reactions



Crystals and structures of NO-generating nitrite reductase (NiR) complexed with NO-decomposing membrane-integrated NO reductase(NOR)

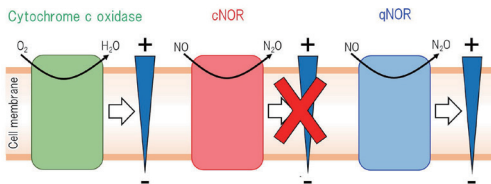
NO transmission path estimated by Molecular dynamics



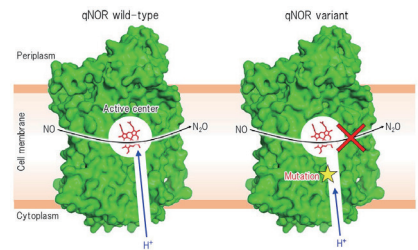
Reference: E. Terasaka *et al.*, *PNAS*, **114**, 9888 (2017)

New antibacterial drug targeting nitric oxide reductase

- Found that decomposing nitric oxide by quinol-dependent nitric oxide reductase (qNOR) generates membrane potential leading to ATP synthesis
- Clarifying the mechanisms of energy conversion and the evolution of respiratory enzymes *in vivo*



Catalytic reaction and membrane potential formation of cytochrome c-dependent NOR (cNOR) and qNOR



Proton transfer route in qNOR deduced from structural and functional analysis



Reference: N. Gonska *et al.*, *Sci. Rep.*, **8**, 3637 (2018)

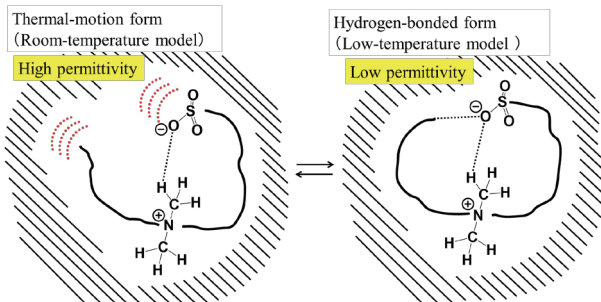
Design for biocompatible materials

- Capturing structural changes due to the formation of weak hydrogen bonding in amorphous biocompatible molecules
- Developing materials sensitive to and compatible with environmental stimuli, such as temperature and pressure

Competition between thermal motion and hydrogen bond formation



Guiding principles for the innovative development of environmental stimuli-sensitive materials



Reference: M. Takahashi *et al.*, *Sci. Rep.*, **9**, 13104 (2019)

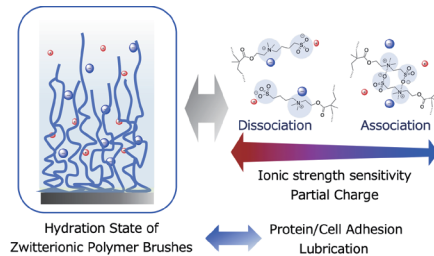
Optimization of material design adjusting to physiological conditions

- Investigated the swelling behavior of zwitterionic polymer brush thin films with a neutral net charge
- Revealed a mechanism of anti-biofouling associated with its interaction with water
- Finding applications related to lubricious and/or anti-biofouling-materials (e.g., artificial joints, artificial blood vessels, artificial hearts, and ECMO)

Zwitterionic Polymer Brushes

- ✓ Neutral net charge
- ✓ Hydrophilicity
- ✓ High osmotic pressure

Interaction with Water



The interaction between the zwitterionic polymer chains and water depends on the charge spacer length in the zwitterions.

Hydration States of Zwitterionic Polymers

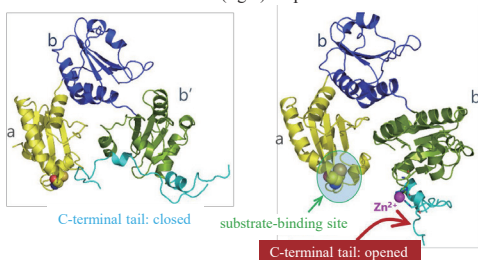


Reference: Y. Higaki *et al.*, *Langmuir*, **33**, 8404 (2017)

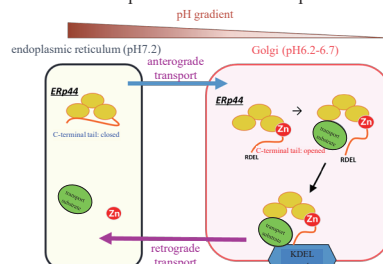
Importance of zinc in cells

- Solved the crystal structures of the pH-sensitive chaperone ERp44 with and without zinc
- Found the uptake of zinc in the Golgi necessary for protein quality control by ERp44
- Discovering a new relationship between constituent elements and functions

Crystal structure of zinc-free (left) and zinc-bound (right) ERp44



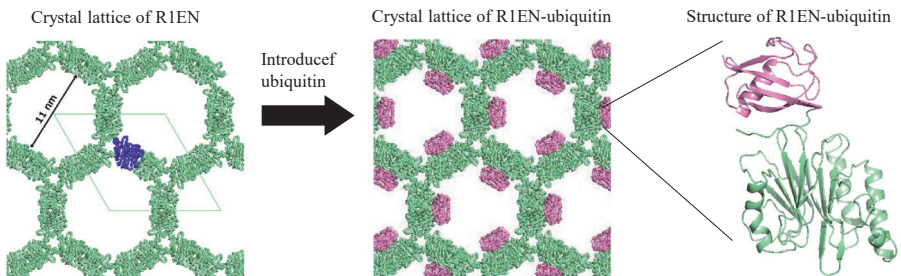
Retrograde transport of abnormal proteins by the cooperation of zinc and ERp44



Reference: S. Watanabe *et al.*, *Nat. Commun.*, **10**, 603 (2019)

■ Development of an innovative protein crystallization method

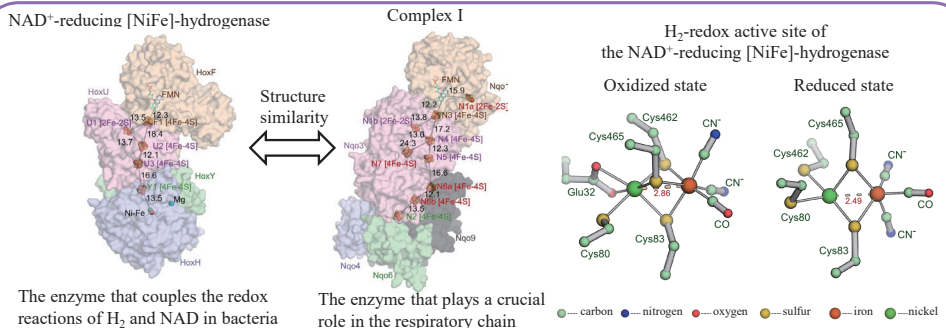
- Structure determination of a target protein (ubiquitin) by genetic fusion to a protein (R1EN), which forms a highly porous crystal lattice of R1EN
- Improving crystal structure analysis for *de novo* proteins



Reference: N. Maita, *J. Am. Chem. Soc.*, **140** (42), 13546 (2018)

■ O₂-attack preventing mechanism of enzymes

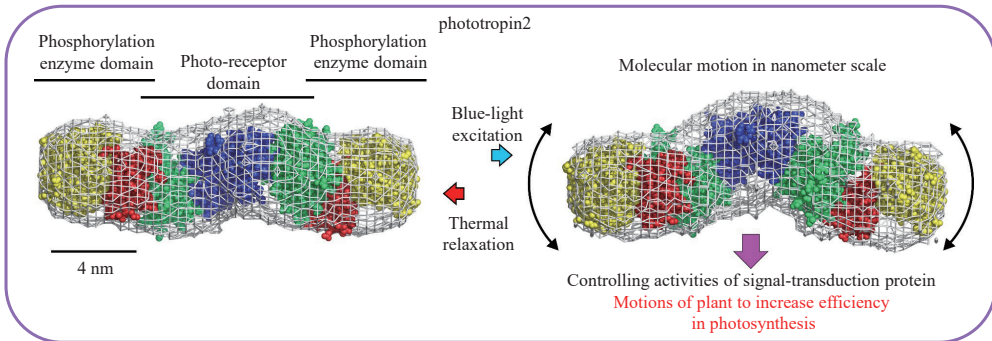
- Analyzed the crystal structures of the NAD⁺-reducing [NiFe]-hydrogenase, which catalyzes the redox reaction of hydrogen in bacteria
- Found electron-transfer cluster functions to be the switch of the conformational change in the H₂-redox active site
- Elucidating the ROS-attack preventing mechanisms that involve the structural changes and molecular evolution of energy metabolism systems



Reference: Y. Shomura *et al.*, *Science*, **357**, 928 (2017)

Increasing efficiency in photosynthesis

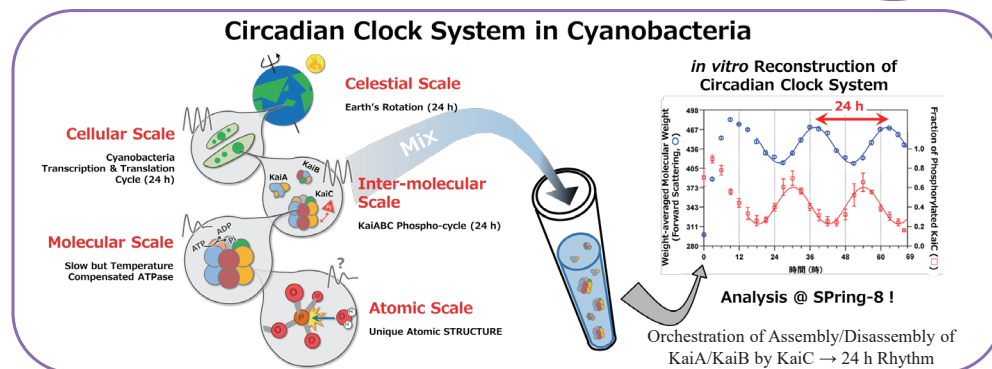
- Studied the molecular structure of the blue-light receptor protein phototropin2 in plants
- Found an enhancement of phosphorylation activity of phototropin2 through conformational change induced by blue-light
- Utilizing biological materials and optogenetics to control gene-expression using light



Reference: Oide *et al.*, *J. Bio. Chem.*, **293**, 963 (2018)

Biological rhythm and dynamics

- Real-time observation of assembly and disassembly dynamics of a cyanobacterial periodosome composed of three kinds of clock proteins (KaiA, KaiB, and KaiC)
- Tracking the circadian rhythms of the cyanobacterial clock protein KaiC
- Understanding design principles for molecular clock oscillators and circadian periods

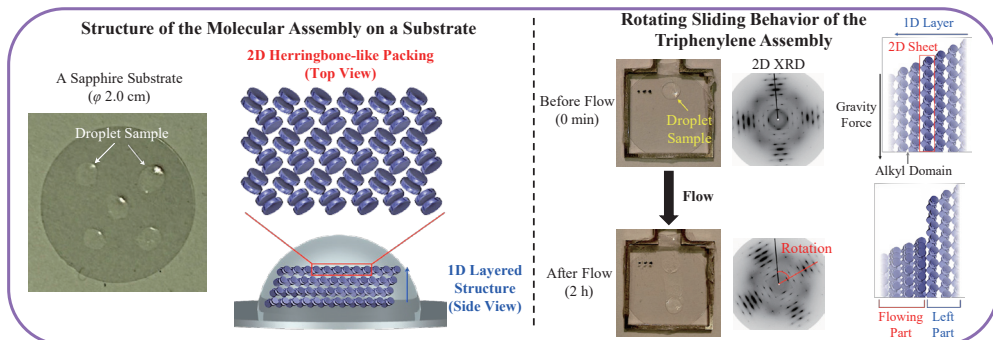


Reference: Akiyama *et al.*, *Mol. Cell*, **29**, 703 (2008)
Maruyama *et al.*, *EMBO J.*, **30**, 68 (2011)

New understanding of molecular self-assemblies

- Spontaneous assembly of a discotic molecule (a triphenylene derivative) created “droplets” with a single-crystal-like 3D structural order, which behaved like both a solid and a liquid and flowed without disrupting its structural order.
- Molecular chirality can control the direction of motion of a macroscopic molecular assembly.

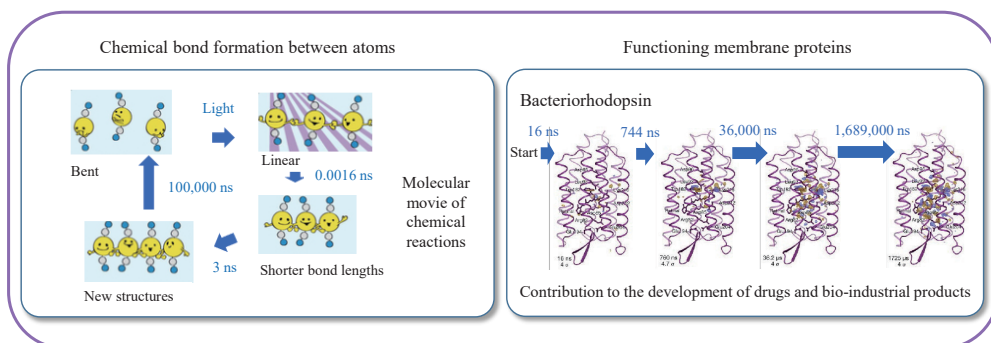
→ Promoting the understanding of structuring and dynamic behaviors of molecular assemblies



Reference: T. Kajitani *et al.*, *Nature Mater.*, **18**, 266 (2019)

Recording molecular movies

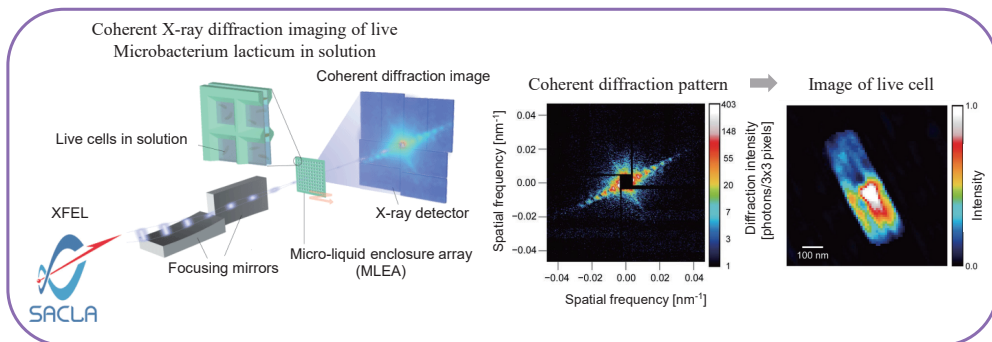
- Observed chemical bond formations
 - Observed functioning membrane proteins
- Designing chemistry composition



Reference: E. Nango *et al.*, *Science*, **354**, 1552 (2016)
K. H. Kim *et al.*, *Nature*, **518**, 385 (2015)

Imaging live cells

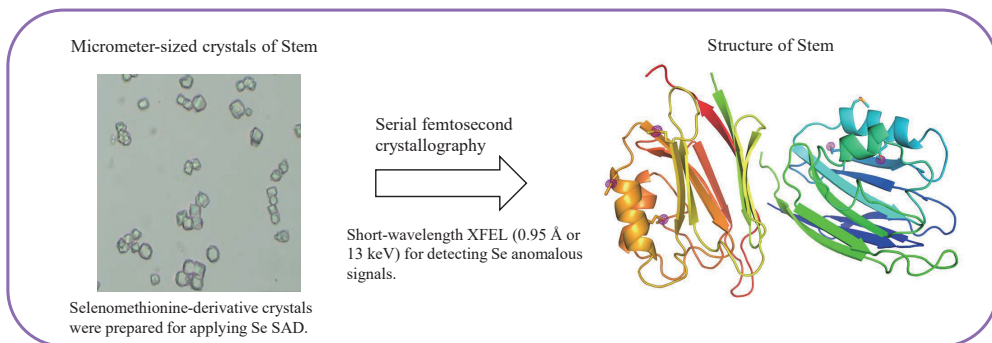
- Visualizing the internal structures of live cells at a nanometer scale
- Contributing to cell biology and medical science



Reference: T. Kimura *et al.*, *Nat. Commun.*, **5**, 3052 (2014)

De novo structure analysis of proteins using short-wavelength XFEL

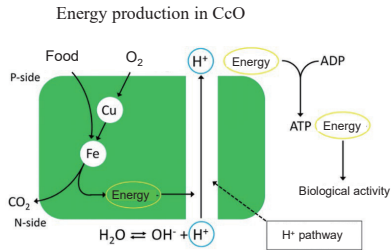
- Applied the single-wavelength anomalous diffraction (SAD) technique to serial femtosecond crystallography
- Determined the structures of selenomethionine-labeled proteins (Stem and ACG) at an X-ray wavelength of 0.95 Å
- Facilitating *de novo* structural determination of biomacromolecules using XFEL



Reference: K. Yamashita *et al.*, *IUCrJ*, **4**, 639 (2017)

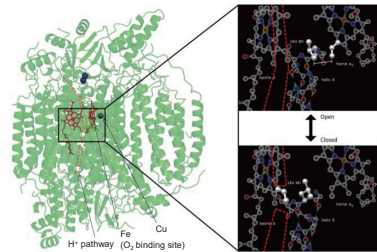
Energy production mechanisms of mammals

- Analyzing structural changes of bovine cytochrome c oxidase (CcO) using time-resolved X-ray crystallography at a nanosecond timescale
 - Revealing the mechanisms for effective proton pumping that produce energy for biological activities
- Understanding respiratory enzyme systems



It remains an open question how CcO blocks backward flow of H^+ .

Structures of pre and post reaction with oxygen



The proton pathway (dashed red lines) is closed after O_2 binds to Cu at the oxygen reduction site.

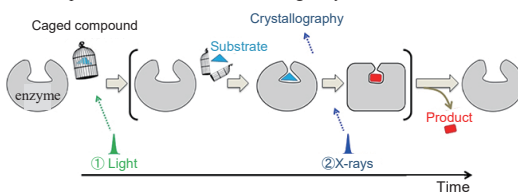


Reference: A. Shimada *et al.*, *Sci. Adv.* **3**, e1603042 (2017)

Visualization of enzymatic reactions

- Atomically resolved structure analysis of enzymes during reaction with substrates by using caged compounds that release substrate molecules upon photoexcitation
- Developing pharmaceuticals through a better understanding of the mechanisms that drive enzymatic reactions

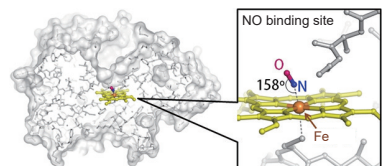
Experimental method for observing enzymatic reactions



Caged compounds release substrate molecules upon photoexcitation, which triggers enzymatic reactions.

Intermediate states are observed by X-ray crystallography.

Fungal nitric oxide reductase (P450nor)



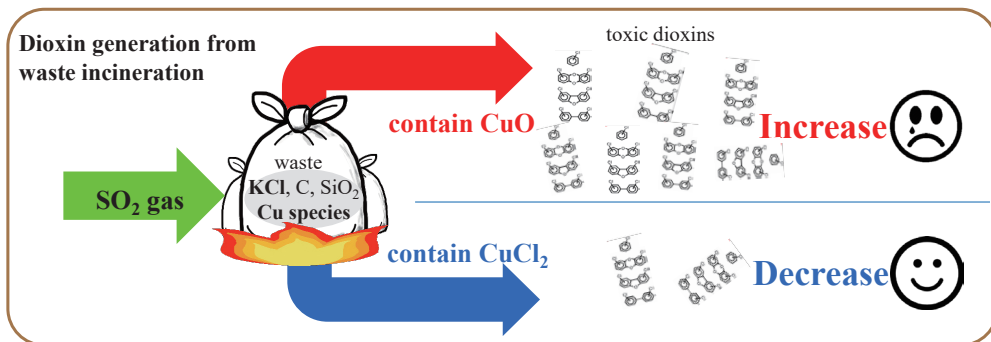
Structure at the moment that P450nor takes in a nitric oxide (NO) molecule as a substrate.



Reference: T. Tosha *et al.*, *Nat. Commun.*, **8**, 1585 (2017)

Waste treatment with less pollution

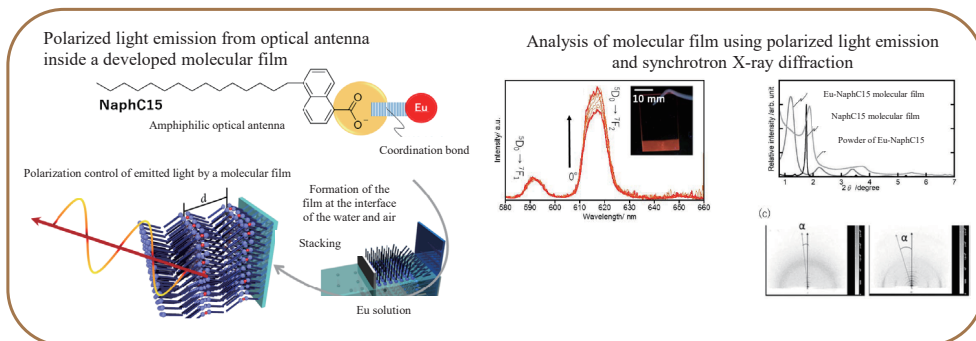
- Understanding the formation mechanisms of dioxins derived from incineration processes
- Inhibiting the generation of toxic dioxins



Reference: T. Fujimori, M. Takaoka *et al.*, *Environ. Sci. Technol.*, **48**, 13644 (2014)

New peep prevention filter

- Inserting a rare-earth film into the stacked soft molecular films of one-atom intervals
- Elucidating the stacked structure by using synchrotron X-ray diffraction and optical waveguide polarization absorption spectrum
- Contributing to the diversity and utility of materials by incorporating polarizing filters into future material designs

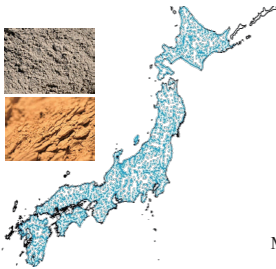


Reference: K. Yoshihara *et al.*, *New J. Chem.*, **43**, 6472 (2019)

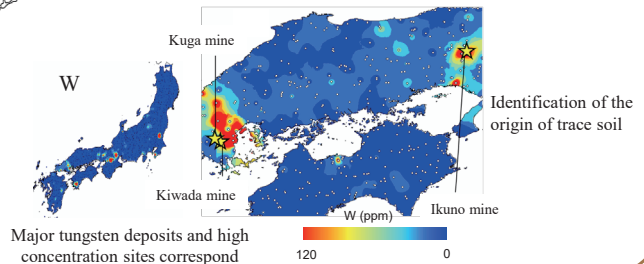
■ Identify sediment-producing areas for forensics

- Completion of a sediment database for all of Japan
- Estimation of areas of production with even a small amount of sediment
- Strengthening and enhancing the forensics field

Analysis of 3024 river sediments



Tungsten (W) distribution map



Reference: N. Nakai *et al.*, *X-ray Spectrometry*, **43**, 38 (2014)

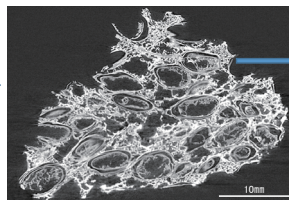
■ Evolution of rice plants by cultivation

- Found unhulled rice from the Yayoi period in excavated rice blocks
- Observed the fine structure of the unhulled rice using X-ray micro-CT
- Understanding the evolution of rice from observing the morphological changes of unhulled rice

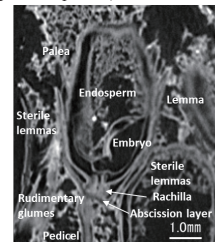
Excavated rice block in the early Yayoi Period



Well-preserved unhulled rice is included in excavated rice block.



Unhulled rice showing morphological change with cultivation (Temperate Japonica)

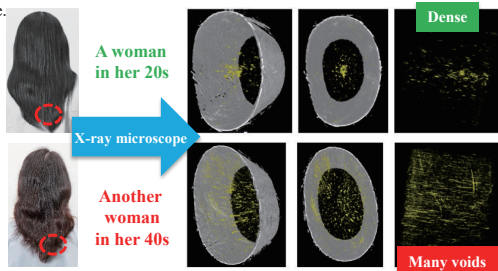


Reference: T. Inamura *et al.*, *Journal of Crop Research*, **61**, 27 (2016)

Hair care for healthy hair

- Investigated 3D structures of isolated hair strands from women of different ages using X-ray microscopy
- Discovered a tendency of the tip of hair strands to have an increase in voids at older ages
- Developing hair-care products “Aujua IMMURISE” that can repair hair

Changes in properties of hair, such as moisture and curly, with aging causes tendency for women to keep their hair shorter because of increased effort in hair care.



The X-ray microscope can visualize fine structures inside hairs as small as ~200 nm in 3D without any preparation.

Voids at the tip of hair increased with age.
New hair care products to repair damaged hair



Milbon Co., Ltd.

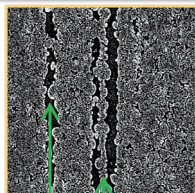
Delicious “tenobe somen” noodles

- “Somen” is a thin Japanese wheat noodle with more than 600 years of history
- The 3D structures of dried noodles made by both traditional “tenobe” (hand-stretching) and machine production were compared using X-ray micro-CT
- Elucidating the structural origins of the noodles’ desirable chewy (koshi) and throat-pleasing (nodogoshi) textures

3D microstructural analysis of dried somen noodles

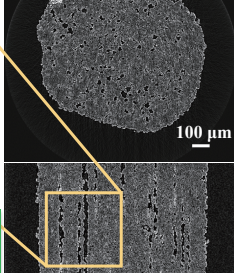


Origin of the unique textures “Koshi” and “Nodogoshi”.

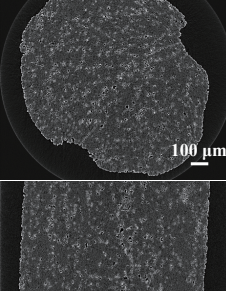


Intact starch granules are supported on bundles of gluteins oriented along stretched direction

“Tenobe” noodle (Hand-stretching production)



Machine production noodle

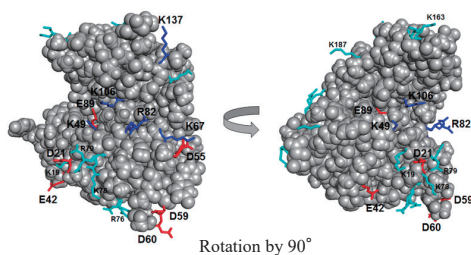


Hyogo Prefecture Tenobe Somen Cooperative, University of Hyogo
Reference: N. Hosoda *et al.*, *J. Cook. Sci. Jpn.*, **52** (6), 386 (2019)

■ Enhancement of sweeteners

- Enhanced the sweetness of thaumatin
 - Elucidated the interaction between sweet receptors and thaumatin
- Developing low-calorie sweeteners and pharmaceuticals

Crystal structure of thaumatin



Enhancement of sweetness and elucidation of its mechanism

- Mutation of an aspartic acid (D21) into asparagine.
- Tethered docking simulation.

For further applications;

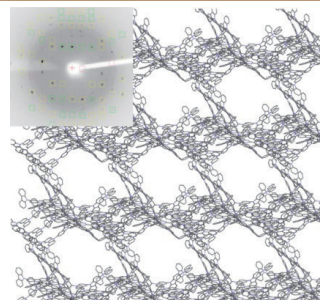
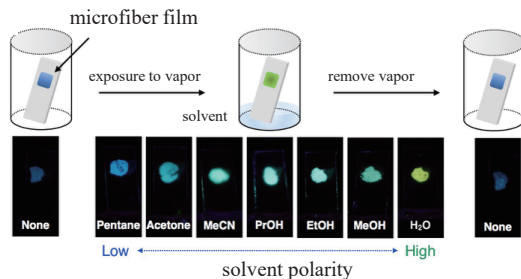
- Low-calorie sweeteners
- Novel seasonings
- Pharmaceuticals



Reference: T. Masuda *et al.*, *Sci. Rep.*, **6**, 20255 (2016)

■ Highly sensitive detection and discrimination of volatile molecules

- Developed a new crystalline framework from a dendrimer
 - Enhanced the photoluminescence of the highly porous structure with color change upon exposure to solvent vapors
- Developing technology for sensing and distinguishing volatile molecules



Crystal structure and X-ray diffraction image



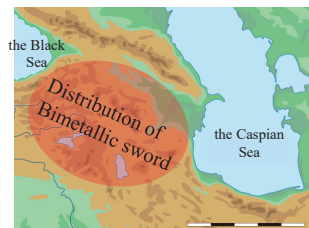
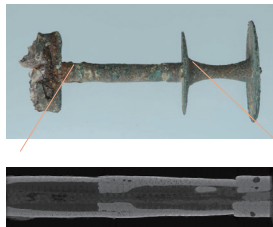
Reference:

S. Nakajima *et al.*, *Chem Comm.*, **54**, 2534 (2018)

Exploring the origin and spread of iron weapons

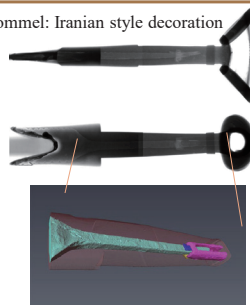
- Took clear X-ray micro CT images of the inside of the hilt of bimetallic swords, made at the beginning of Iron age
- Discovered that the method for making the bimetallic sword, an iron sword with a bronze hilt, was “cast-in” technology with two other metals
- Providing new evidence for the spread of iron weapons incorporated with the bronze casting system, prior to the development of iron forging technology

Pommel: Caucasian style decoration



Iron weapons became popular as “prestige” with bronze pommel reflecting local culture.

Pommel: Iranian style decoration

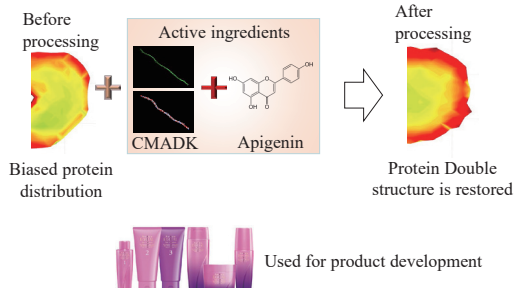
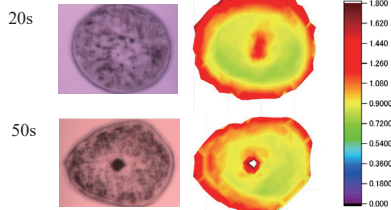


Reference: R. Shikaku *et al.*, The 11th ICAANE (2018)

Recovery of hair root collapse due to aging

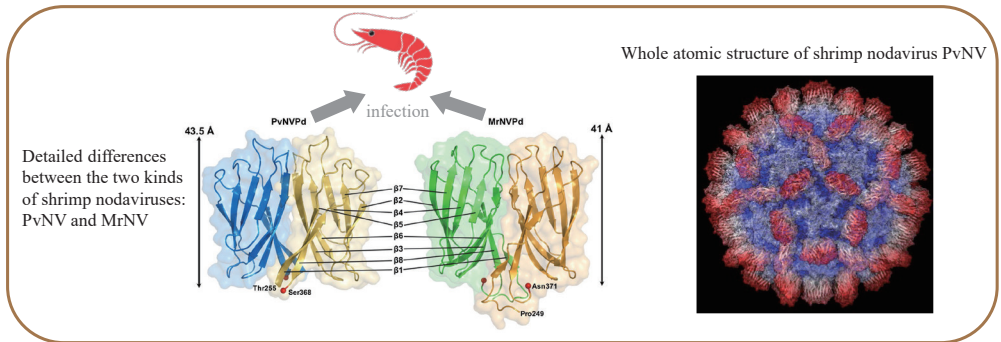
- Analysis of structural differences in strands of hair as a human ages
- Repairing hair with active ingredients

Aging disrupts the dual structure of proteins, resulting in a biased distribution



More efficient shrimp aquaculture

- Elucidation of the atomic structures of shrimp nodavirus
- Determination of detailed structures of shrimp nodaviruses, PvNV and MrNV, at high resolution
- Revealing the infection mechanisms of shrimp and finding appropriate countermeasures



Reference: N.-C. Chen *et al.*, *Commun. Bio.*, 2, 72 (2019)

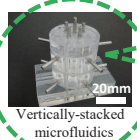
Highly sensitive detection of endocrine-disturbing chemicals in the sea

- Development of an environmental analysis system with extremely high sensitivity based on vertically-stacked microfluidics
- Development of a basic platform for three-dimensional micro fluidic networks
- Developing sequential unit chemical operations with a high rate and yield, utilizing 3D microfluidic behavior and size effects

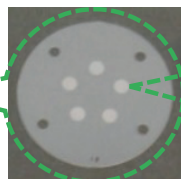
High sensitivity detecting of endocrine disturbing chemicals in sea was successfully demonstrated with the sensitivity of decades fold as so far by using a novel vertically-stacked reactor, in which cross-linked capillaries were immobilized by antibody.



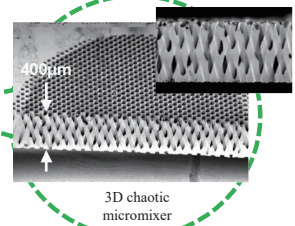
Extremely high sensitive environmental analysis system



Vertically-stacked microfluidics



Microreactor bundle



3D chaotic micromixer



Reference: Y. Utsumi *et al.*, *Sensors and Actuators B*, 166-167, 898 (2012)

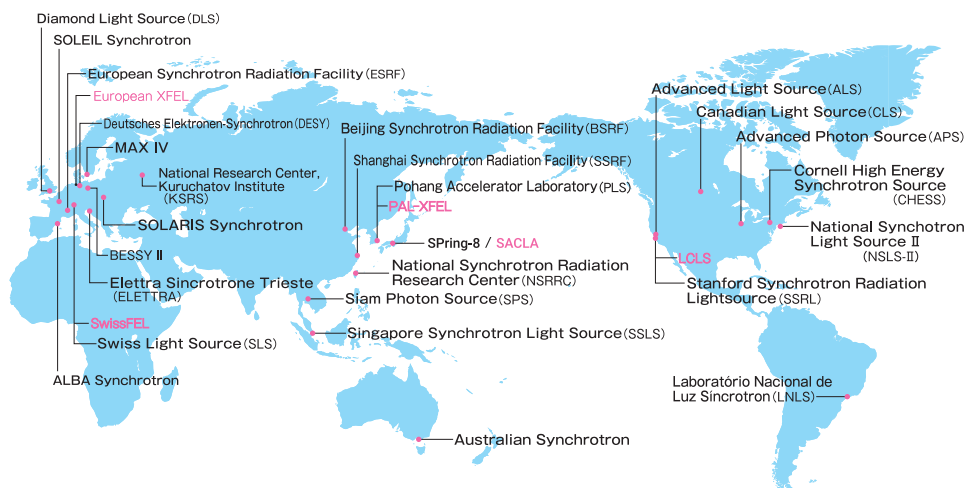


Synchrotron Facilities around the World

Synchrotron radiation (SR) facilities generate intensive X-rays resulting from high-energy electrons.

The X-rays are utilized to observe the atomic/molecular world. Among the many SR facilities in Japan and around the world, SPring-8 and SACLA provide the highest levels of capabilities.

Synchrotron Facilities around the World

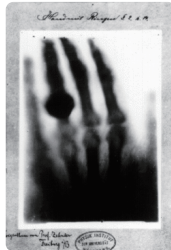


Synchrotron Facilities in Japan





Introduction to X-rays

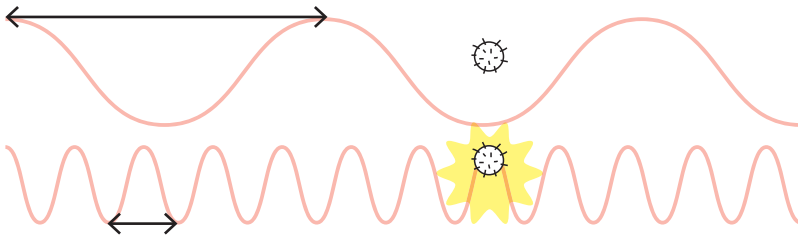


In 1895, Röntgen discovered a type of light able to penetrate materials.

The X-rays were named after the 'X' used in mathematics to designate an unknown variable. The first X-ray image was the hand of his wife. Now X-rays are widely used in hospitals.

We are able to see objects with light.

Shorter wavelength light allows us to see smaller objects limited by wave length.



Although light with a longer wavelength cannot image small objects, light with a shorter wavelength can. (X-ray wavelength is approximately atomic size)

Terahertz	Infrared	Visible	Ultraviolet	VUV	Soft X-ray	Hard X-ray
100 μm	10 μm	1 μm	100nm	10nm	1nm	0.1nm

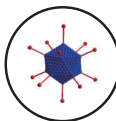
longer $\longleftarrow$ wavelength of light $\longrightarrow$ shorter



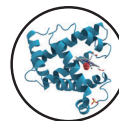
Hair



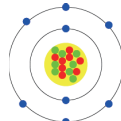
Bacteria



Viruses

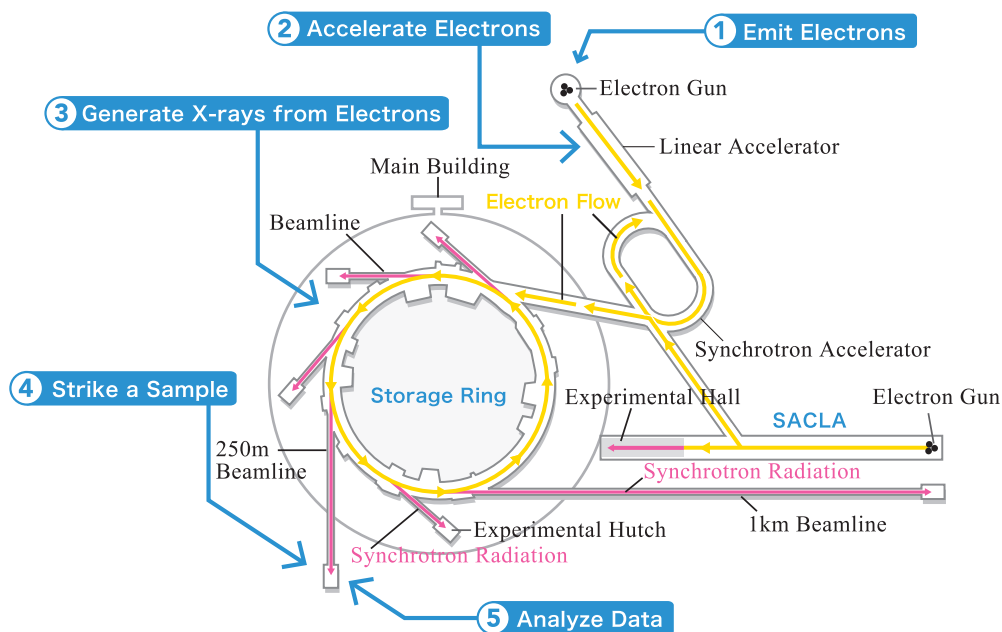


Proteins



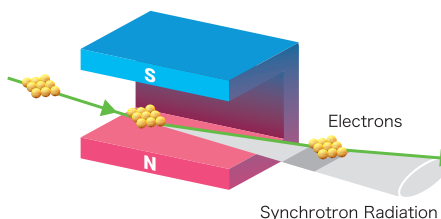
Atoms

SPRING-8 can image small objects that have never been observed before by using very intense X-rays from a large accelerator.



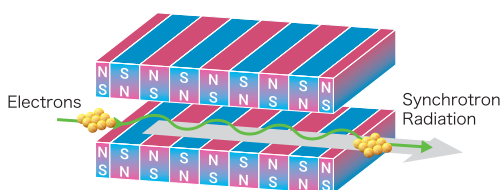
How to Generate Synchrotron Radiation

1 Bending Magnet



Bending of an electron trajectory causes radiation toward its tangential direction. Electrons at higher speeds generate X-rays with shorter-wavelengths.

2 Undulator



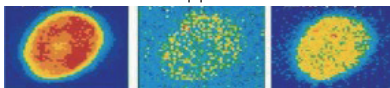
Bending electron trajectories multiple times by magnetic fields generates strong X-rays in a forward direction. Shorter wavelengths of X-rays can be achieved by increasing the speed of the electrons and by using undulators with a shorter period.

How to observe small structures that we cannot view with our eyes alone

Various phenomena in light-matter interactions

Observe elements

Sulfur Copper Zinc



Analysis of elements in the cross-section of a hair

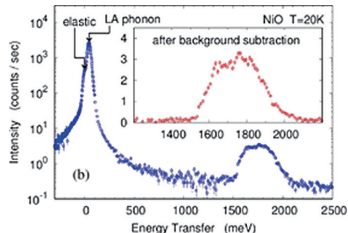
X-ray Fluorescence Analysis

Measure electrons emitted from materials excited by X-rays

X-ray Inelastic Spectroscopy

Measure the energy shift of X-rays
Observe nanodynamics in materials

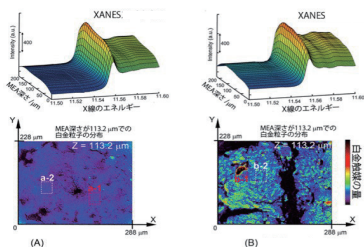
Direct observation of scattered X-rays



X-ray Absorption Fine Structure (XAFS)

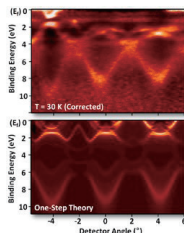
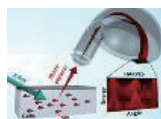
Measure X-ray absorption

Observe chemical states



Distribution of platinum catalysts in an MEA cathode catalyst layer of a fuel cell

Observe energy states



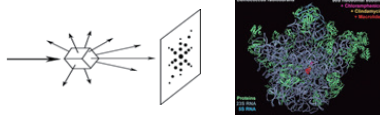
Photoemission Spectroscopy

Measure X-rays radiated from materials that have absorbed X-rays

Photoelectron Spectroscopy

Measure the energy of electrons emitted from materials irradiated by photons

Observe atomic and molecular structures



Imaging

Observe transmitted X-rays

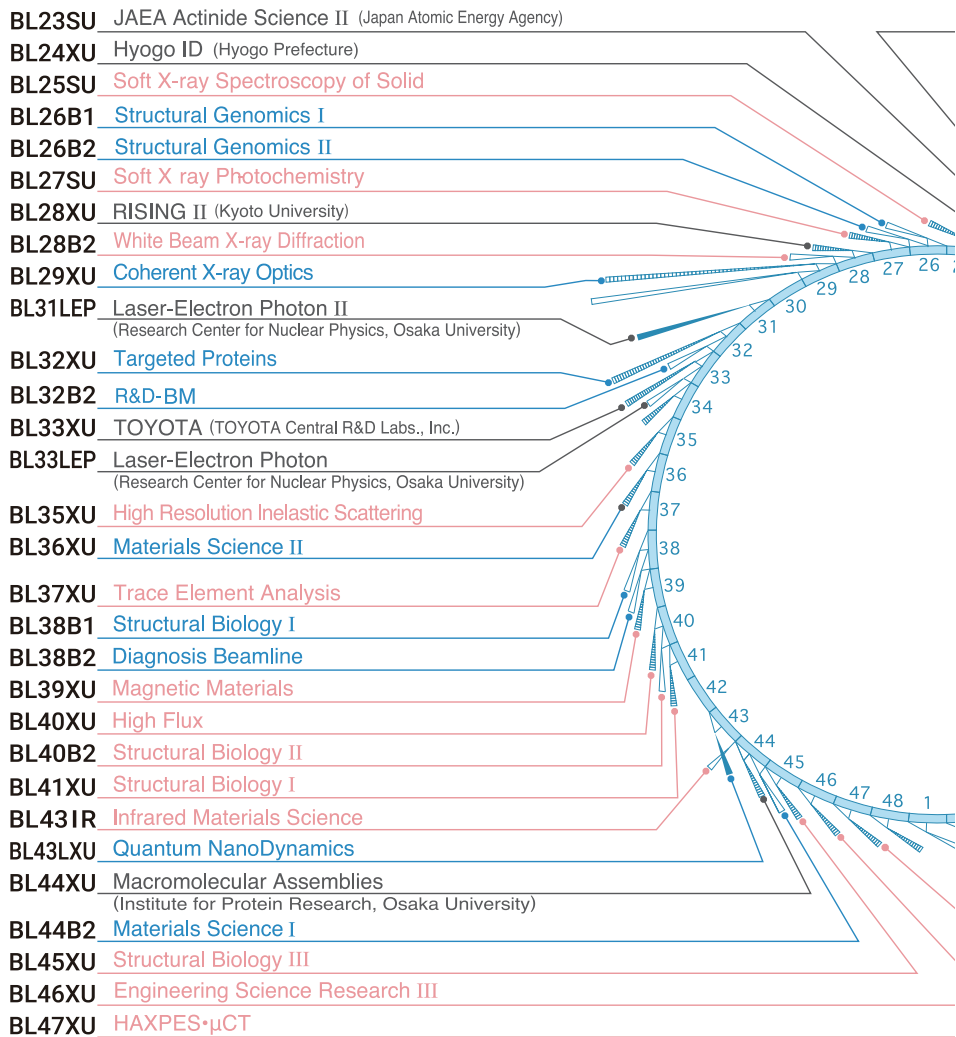
Visualize see-through bodies



The air penetrating process in new born rabbit's lungs



Beamline Map



Notes for beamline abbreviations

XU (Hard X-rays by undulators)

SU (Soft X-rays by undulators)

B1/B2 (Bending Magnets)

Hard X-rays with high brilliance that are generated by in-vacuum undulators

Soft X-rays that are generated by undulators with a long magnetic period

Broadband X-rays that are generated by bending magnets

JAEA Actinide Science I (Japan Atomic Energy Agency) BL22XU

Medical and Imaging I BL20B2

Medical and Imaging II BL20XU

Engineering Science Research I BL19B2

SR Physics BL19LXU

Coherent Soft X-ray Spectroscopy BL17SU

SUNBEAM BM BL16B2

(SUNBEAM Consortium)

SUNBEAM ID BL16XU

(SUNBEAM Consortium)

WEBRAM BL15XU

(National Institute for Materials Science)

Engineering Science Research II BL14B2

QST Quantum Dynamics II BL14B1

(National Institutes for Quantum and Radiological Science and Technology)

Surface and Interface Structures BL13XU

NSRRC BM BL12B2

(National Synchrotron Radiation Research Center, Taiwan)

NSRRC ID BL12XU

(National Synchrotron Radiation Research Center, Taiwan)

QST Quantum Dynamics I BL11XU

(National Institutes for Quantum and Radiological Science and Technology)

High Pressure Research BL10XU

Nuclear Resonant Scattering BL09XU

Hyogo BM (Hyogo Prefecture) BL08B2

High Energy Inelastic Scattering BL08W

The University-of-Tokyo Outstation Beamline for Materials Science BL07LSU

(The University of Tokyo)

R&D-ID BL05XU

High Energy X-ray Diffraction BL04B2

High Temperature and High Pressure Research BL04B1

Advanced Softmaterial BL03XU

(Advanced Softmaterial Beamline Consortium)

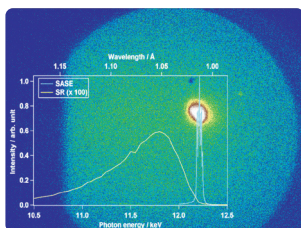
Powder Diffraction BL02B2

Single Crystal Structure Analysis BL02B1

XAFS BL01B1

Public Beamlines
Contract Beamlines
RIKEN Beamlines

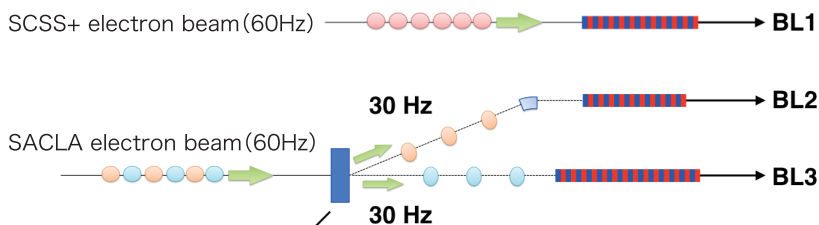
SACLA is an X-ray free electron laser facility that enables us to visualize ultrafast phenomena such as chemical reactions. The motion of atoms and molecules can be seen more clearly than ever by using the intense coherent X-rays of SACLA.



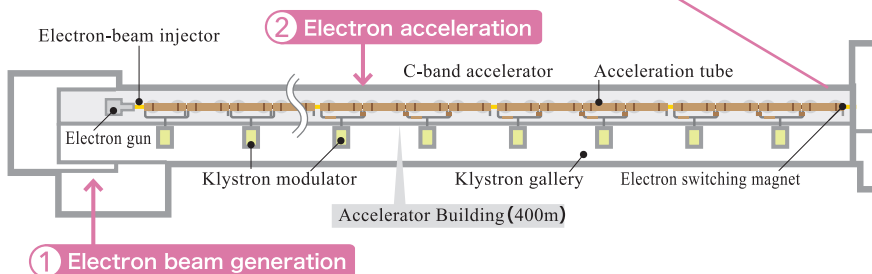
SACLA lased on June 7, 2011 and achieved the world's shortest wavelength of 1 angstrom.

Parallel Operation Of 3 Beamlines

Experiments can be performed simultaneously at the 3 beamlines.



The electron switching magnet distributes electron bunches to 2 beamlines in a pulse-by-pulse manner.



Soft X-ray Free Electron Laser

Only SACLA !

Two independent soft X-ray and hard X-ray lasers operate in the same facility.

The soft X-ray laser is utilized to reveal the mechanisms of phenomena such as catalysis and photolithography.

Prototype
SCSS test accelerator (~2013)



SACLA BL1 (2015~)

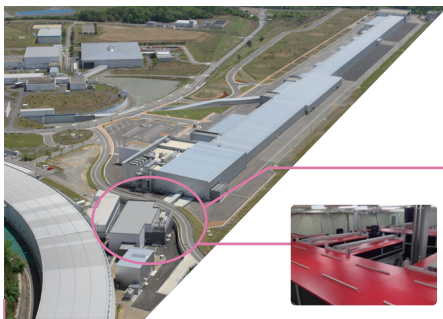


XFEL-SPRING-8 Experimental Facility

High power optical lasers generate extreme states of matter, which are probed by XFEL of SACLA.

There are applications for a wide variety of research fields:

- High energy density science
- Laser acceleration
- Nuclear physics
- X-ray quantum optics

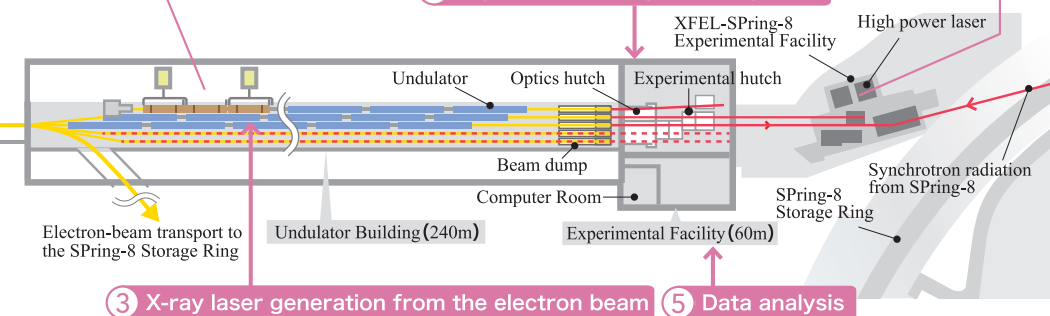


Interaction chamber



Two
500,000,000,000,000-W
laser systems

④ Experiments using the X-ray laser



Remarkable Characteristics of SACLA

SACLA has produced important research results by taking advantages of these three major capabilities.

① Highly Coherent Visualize native structures with precision

Coherent and ultrashort X-ray pulses of SACLA give clear sample images in an exposure of femtoseconds. This capability can be utilized for accessing native structures of the samples by outrunning radiation damage. In conventional X-ray experiments, the radiation damage obscures the nature of the samples.

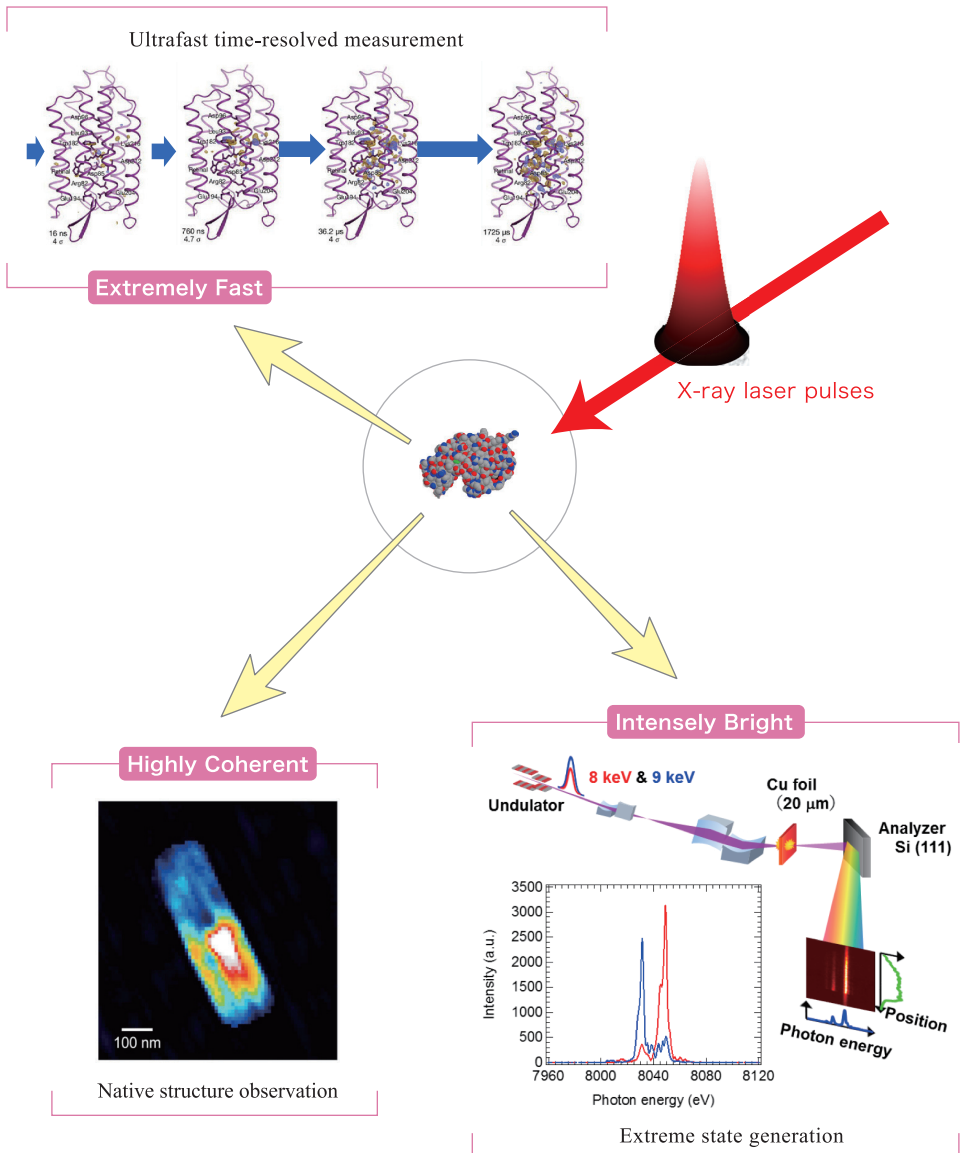
② Extremely Fast Observe rapid phenomena with ultrafast flash

Ultrashort X-ray pulses of SACLA can probe atomic motions in samples, and materials changing fast. This capability is useful for revealing, for example, the mechanism of photosynthesis, development of phase transitions in solid-state materials, and destruction processes of materials.

③ Intensely Bright Generate previously inaccessible states of matter

Ultra intense X-ray pulses of SACLA can generate absolutely unique states of matter. This capability can pave the way for exploring new phenomena that have never occurred in the framework of existing technologies.

Exploring Previously Inaccessible Phenomena Using an X-ray Laser



SPring-8 and SACLA in the Future

This booklet presents the press released results from SPring-8 and SACLA related to the SDGs over the last two years. While we have not closely followed the SDGs, SPring-8 and SACLA have made significant contributions to the goals.

We hope that this booklet will serve as a guide for users to align their research objectives to the SDGs. We are expecting SPring-8 and SACLA to help expand Japan's contributions to the SDGs.

While SPring-8 and SACLA have made substantial contributions to the SDGs, there remains much room for improvement in terms of the sustainability of the facilities themselves. The RIKEN SPring-8 Center has ongoing R&D initiatives to increase sustainability for the SPring-8 and SACLA facilities. So far, we have reduced energy consumption by upgrading the lighting in the experimental hall to LEDs and changing the injection system to direct injection from the SACLA linear accelerator.



We are studying how to make our facility even more sustainable. For example, by reducing the stored electron energy of SPring-8 from the current 8 GeV to 6 GeV, we can further significantly reduce our power consumption. Replacement of some electromagnets in the storage ring with permanent magnets leads to the reduction of both power consumption and heat generation. This replacement lessens the demand for cooling water and air conditioning and consequently reduces overall energy consumption.

We expect SPring-8 will be reborn as a light source that is about one hundred times brighter than its current state by changing the accelerator lattice. We call this new light source, 'SPring-8-II'. Once the SPring-8-II upgrade has completed, our ability to contribute to the SDGs will be significantly higher than with our current infrastructure.

SPring-8 and SACLA will continue to contribute not only to the SDGs but also to the sustainable development of humankind. We look forward to your continued support with our state-of-the-art science and technology.

