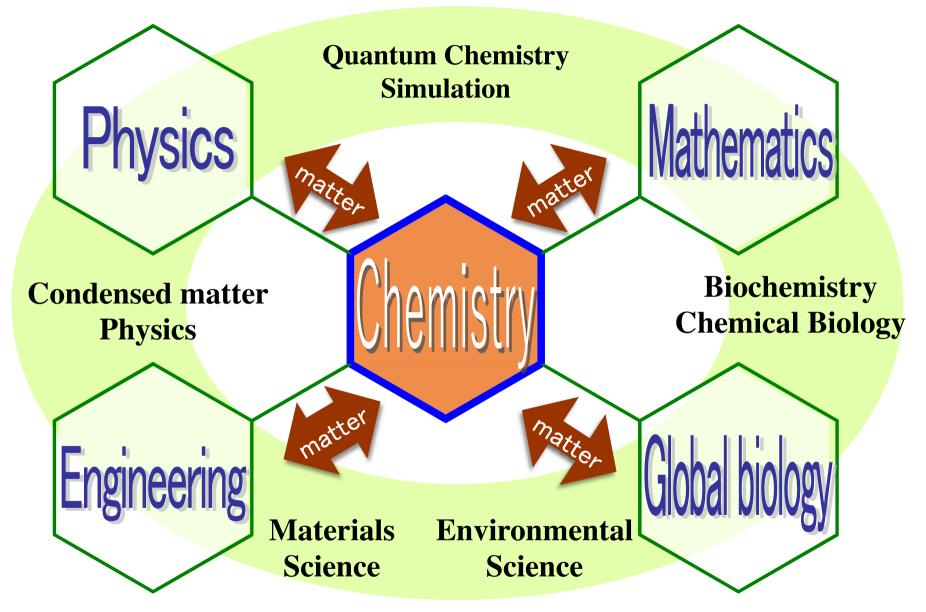
#### Degree Programs in Pure and Applied Sciences, Graduate School of Science and Technology, University of Tsukuba

# Master's/Doctoral Program in Chemistry

https://program.chem.tsukuba.ac.jp/



Chemistry is "Heart of Science", because it studies matter, its composition, and its changes. **( Design, Synthesis, Properties, Funnctions )** 

# CAMIST "artificer" for creating molecules and substances

### "What is a chemical bond?"

It should be important to understand "how the chemical bonds are created".

Handles substances with a well-defined structure

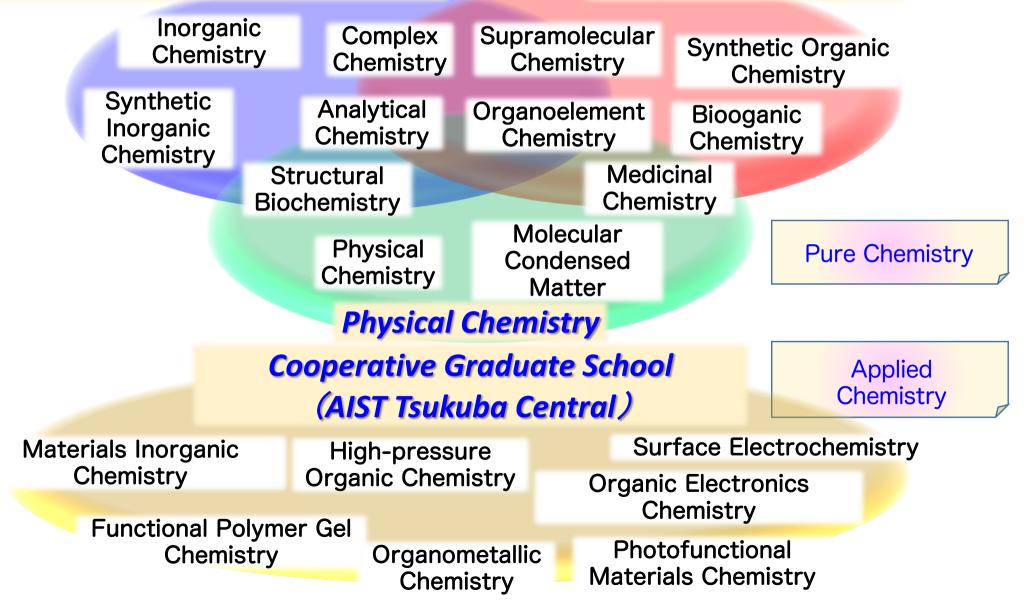
One molecule, a group of substances changes the world

Creating the basis of a material society

#### **Research Fields in Degree Program of Chemistry**

#### Inorganic/Analytical Chemistry

#### **Organic Chemistry**

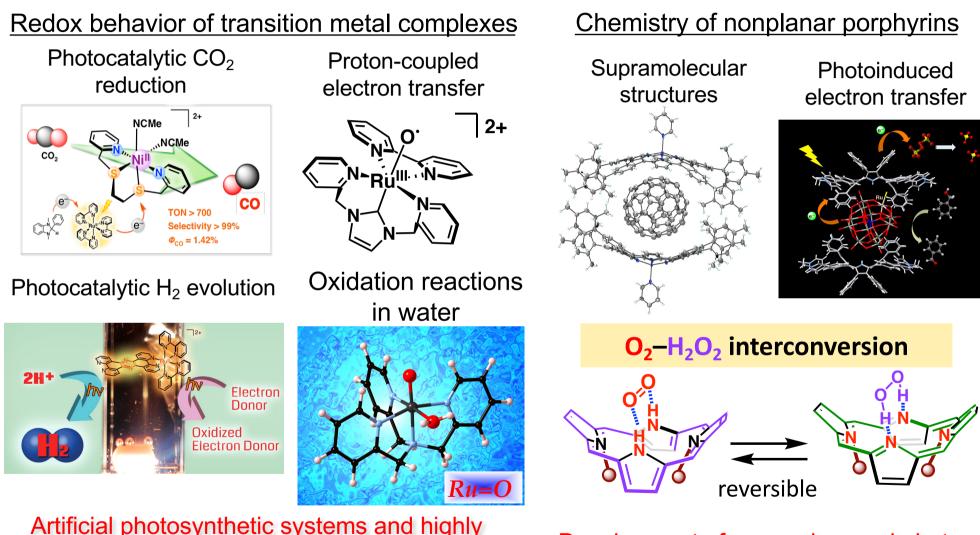


### **Research Fields in Degree Program of Chemistry**

Research Field	Professor	Research
Inorganic Chemistry	Takahiko KOJIMA	Synthesis of transition-metal complexes and their reactivity in various redox and catalytic reactions; supramolecular redox chemistry of non-planar and fused porphyrins.
Analytical Chemistry	Kiyoharu NAKATANI	Studies on chemical processes at microdroplet/solution and microparticle/solution interfaces using electrochemical and spectroscopic techniques.
Synthetic Inorganic Chemistry	Masayuki NIHEI	Creation of multi-nuclear metal clusters with controlled structures and electronic states; chemistry of functional metal complexes with controlled electronic states and structures.
Molecular Condensed Matter	Kazuya SAITO	Structure and property of soft molecular systems, and dynamics and phase transitions in them.
Physical Chemistry	Taka-aki ISHIBASHI	Studies on interfaces and condensed phases by linear and nonlinear molecular spectroscopy; Synthesis of emissive compounds and kinetic analyses of formation and deactivation processes of the emissive state by TCSPC; Studies on photofunctions and photochemical properties of newly fabricated molecular assemblies and inorganic particles in mesoscopic scale.
Bioorganic Chemistry	Hideo KIGOSHI	Isolation, structural elucidation, synthesis, and bioorganic studies of bioactive natural products. Design, synthesis and biological evaluation of novel biologically active molecules.
Organoelement Chemistry	Takahiro SASAMORI	Low-coordinated and multiple-bonded compounds of heavier group 14 elements and organoelement chemistry of Group 13-15.
Supramolecular Chemistry	Takashi NAKAMURA	Precise construction of functional molecules based on supramolecular chemistry, and exploration of their properties such as molecular recognition and selective reaction. Studies on supramolecular metal complexes utilizing organic ligands and metal ions.
Structural Biology and Chemistry	Kenji IWASAKI	Study of proteins in soft-tissue sarcoma, chromatin remodeling factors and a photosensing flavoprotein. Structural biology and chemistry using single-particle electron microscopy and its development.
Medicinal Chemistry	Noriki KUTSUMURA	Design and synthesis of orexin receptor agonists/Design and synthesis of opioid ligands/Research and development for narcorepsy, severe pain, depression, pollakiurea, malaria, other protozoal diseases, and cancer drugs.

# Inorganic Chemistry Lab (Kojima Lab)

### **Bio-inspired Redox Chemistry**

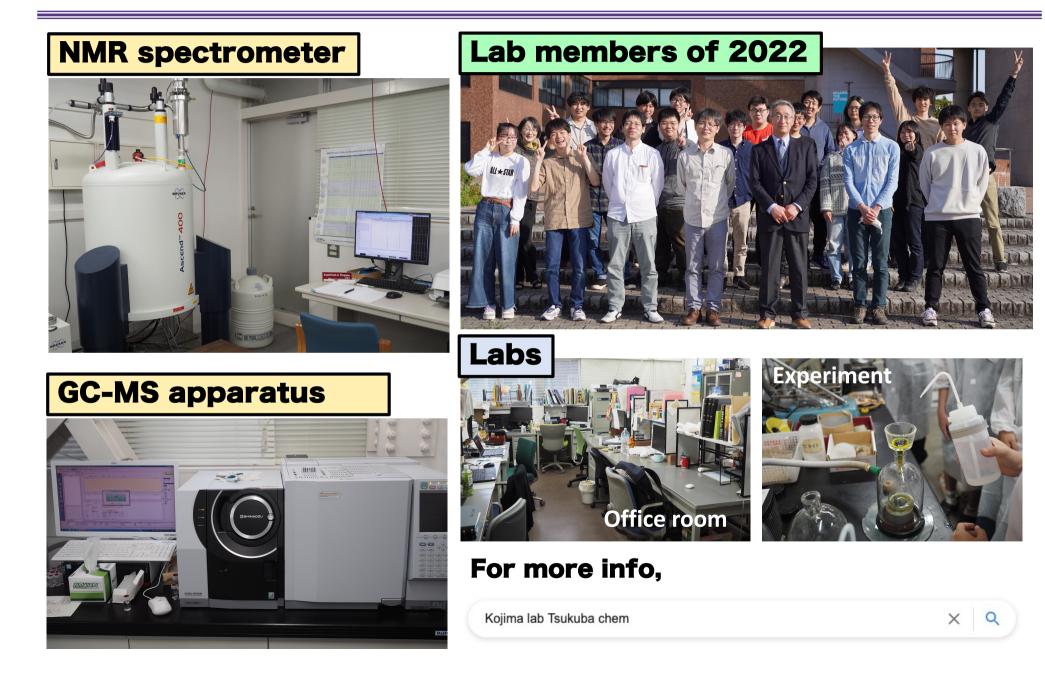


Artificial photosynthetic systems and highly selective oxidation systems based on bio-inspired transition-metal complexes as catalysts

Development of new redox- and photofunctionality based on nonplanar porphyrins

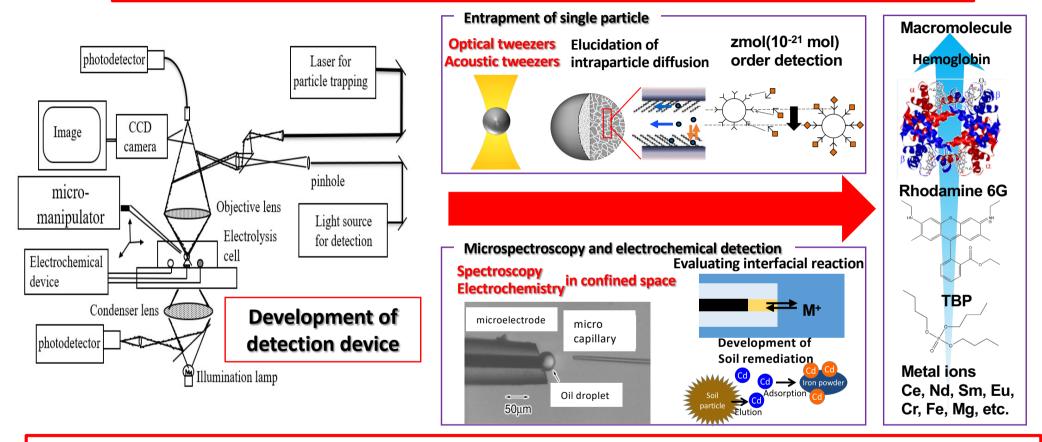
Contact: Takahiko Kojima: 029-853-4323; kojima@chem.tsukuba.ac.jp

# Labs, Equipment, and Lab members



### Analytical Chemistry (Nakatani Lab.)

### Analytical Chemistry based on micro/nano-sized particle



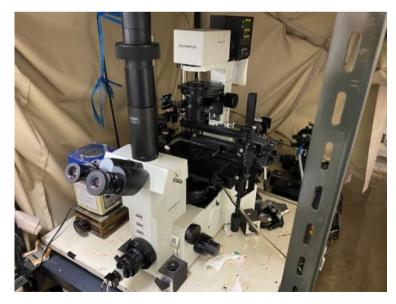
Development of detection device according to target and phenomenon

- Chemical process at interface of the particle and inside the particle
- Separation mechanism of minor actinide from highly active liquid waste
- Regulation and expression mechanisms of oxygen affinity in hemoglobin
- Development of novel detection scheme for proteins and DNAs

#### Synchrotron radiation (X-ray) system



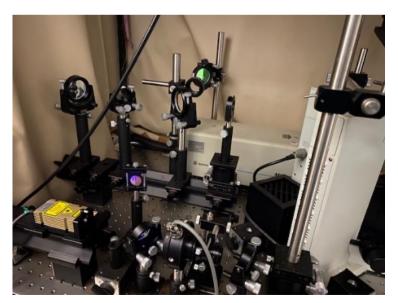
#### Microspectroscopy



#### Detection devices based on ultrasound



#### Optical system for spectroscopy



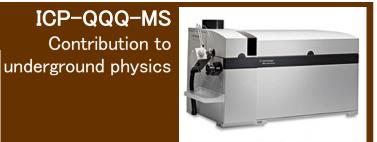


**Ge-semiconductor** Essential for radiation measurements



Counting ultra trace amount of atoms





World-class analytical instruments for ultra-sensitive and accurate analysis Instrumental Analysis Biological experiments

From biology to heavy elements
Lab Experiments

#### Nuclear/Radiochemical approaches to Environmental Analytical Chemistry



アイソトープ環境動態研究センター CRIED CENTER FOR RESEARCH IN ISOTOPES AND ENVIRONMENTAL DYNAMICS

Aya SAKAGUCHI ayaskgc@ied.tsukubai.ac.jp

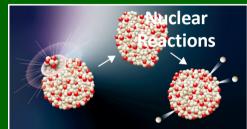
#### The whole planet is a laboratory! Field Work



coral, sediments, seawater



Chemical separation



Production of new isotopes

Kazakhstan Survey

Pu and U contamination



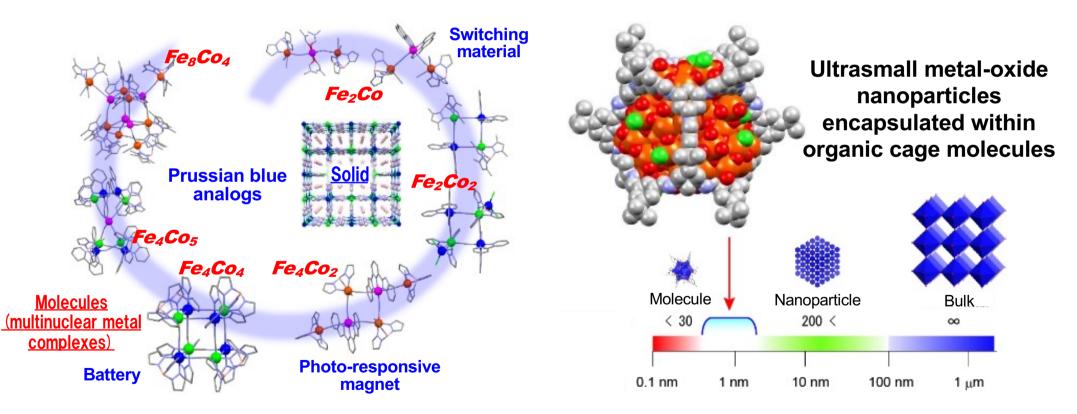
Bucket chemistry

### Synthetic Inorganic Chemistry Lab (Nihei Lab)

Prof. Masayuki NIHEI, Assoc. Prof. Takuya SHIGA, Assist. Prof. Nozomi MIHARA

#### Molecular units of inorganic solid —Emergence of unique properties—

The world's smallest metal oxide nanoparticles (Diameter : 1-2 nm)



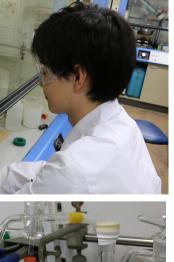
Innovative Molecular Functions Based on Rational Control of Intramolecular Electron Transfer

# Exploration of new chemistry at the boundary of molecules and nanoparticles

### Synthetic Inorganic Chemistry Lab (Nihei Lab)



Organic/inorganic synthesis







Atomic force microscopy

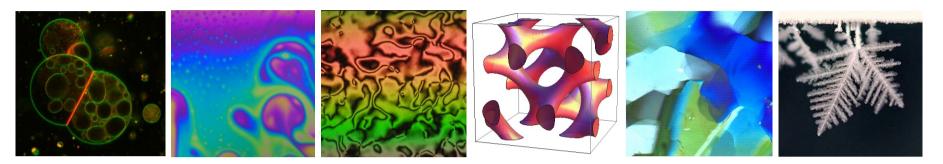


Single crystal X-ray diffraction

Energy dispersive X-ray spectroscopy



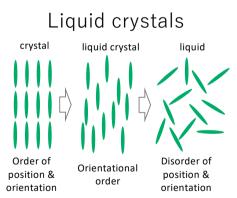
# Molecular Condensed Matter Lab



Soft Matter: Liquid crystals, amphiphilic compounds

Hard Matter: Molecular crystals

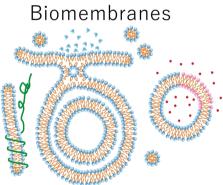
### Relation between "Tree(s)" and "Forest"?



Solid, liquid, and gas are three well-known forms of matter. Liquid crystals have intermediate properties between solid and liquid and are indispensable for modern displays.

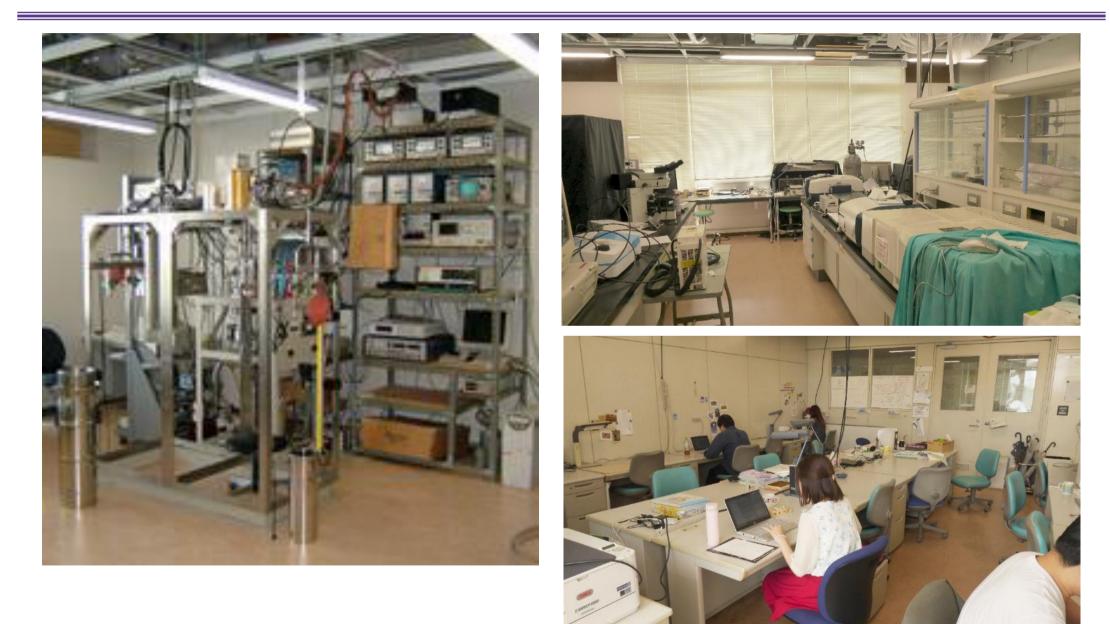


Properties of matter around us depend on the shape and properties of constituent molecules. We pursue an understanding of the relations between molecular and bulk properties. Our research subject ranges from molecular crystals through liquid crystals to colloidal suspensions of membranes.



Cell membranes are made of amphiphilic molecules known as phospholipids. Physicochemical properties of lipid membranes govern their geometry and biological functions.

### Molecular Condensed Matter Lab





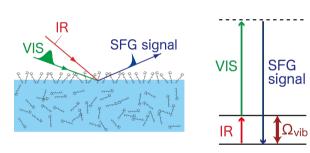
# **Physical Chemistry Laboratory**

Ishibashi Group: Taka-aki Ishibashi, Masato Kondoh, Yuki Nojima

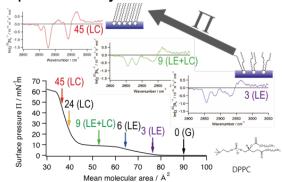
Physical Chemistry of interfaces and solution phase by various spectroscopic techniques

### Surface VSFG

Molecules at interfaces are selectively probed by nonlinear spectroscopy



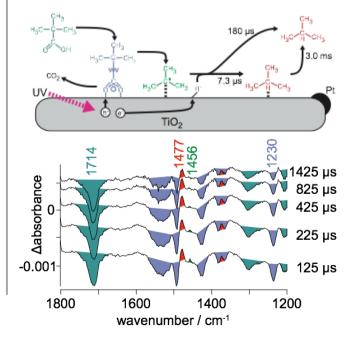
VSFG spectra of lipid monolayers on water



#### Time-resolved IR

Short-lived chemical species are traced by IR spectroscopy

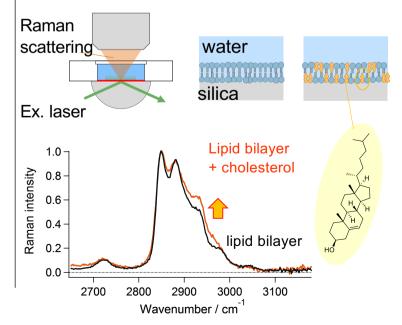
A photocatalytic process on TiO<sub>2</sub> studied by TR-IR

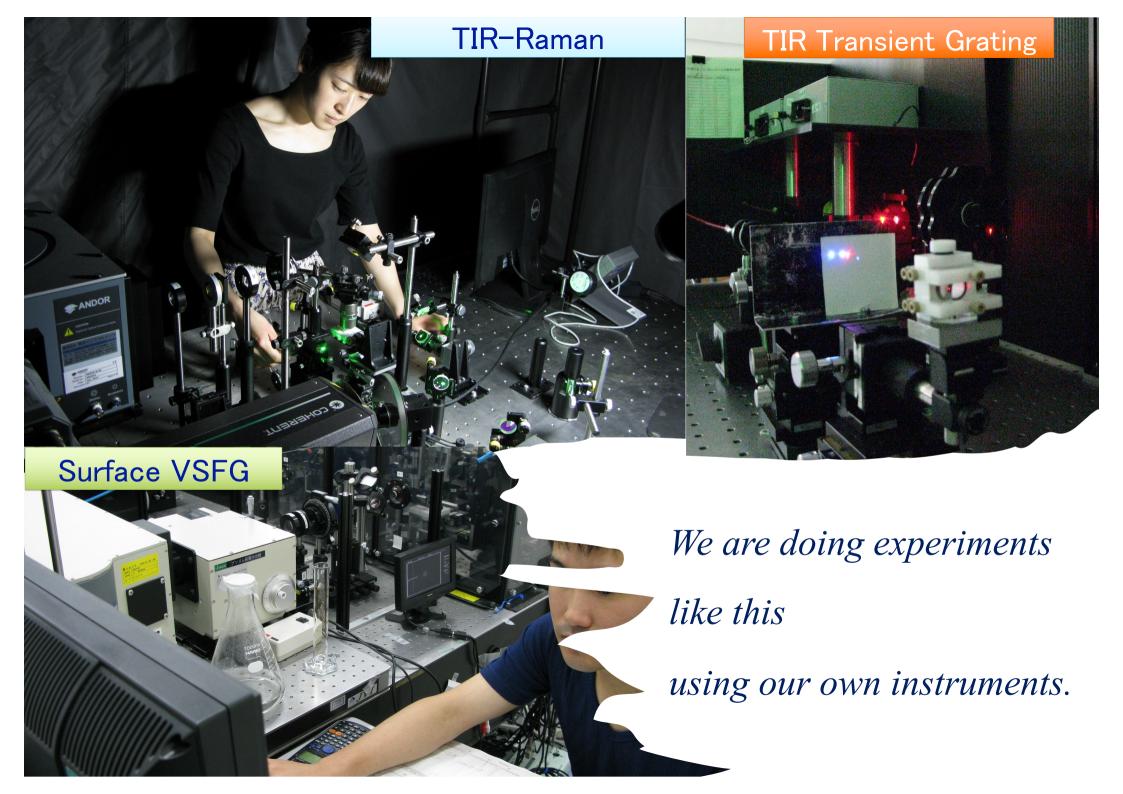


#### TIR-Raman

Total Internal Reflection geometry allowed interface sensitive observation by Raman

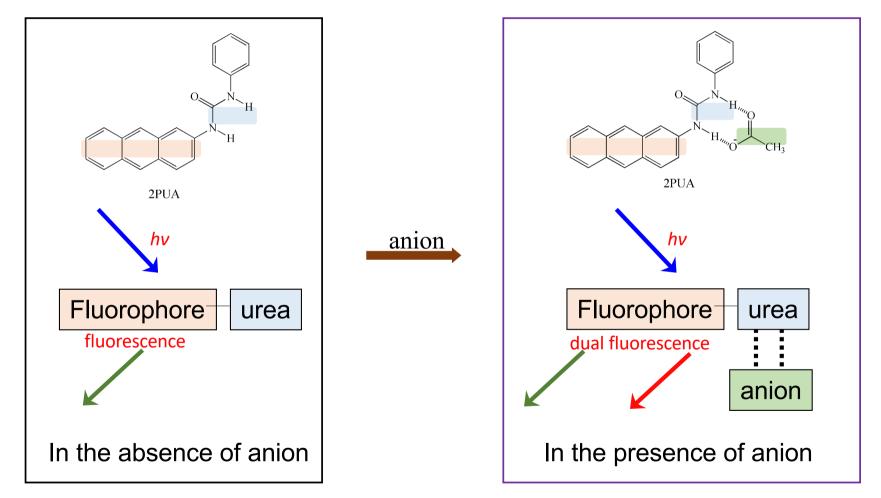
Supported lipid-bilayers + cholesterol probed by TIR-Raman





#### Nishimura Group: Associate Prof. Yoshinobu Nishimura

Anion recognition by fluorescent aromatic urea compounds

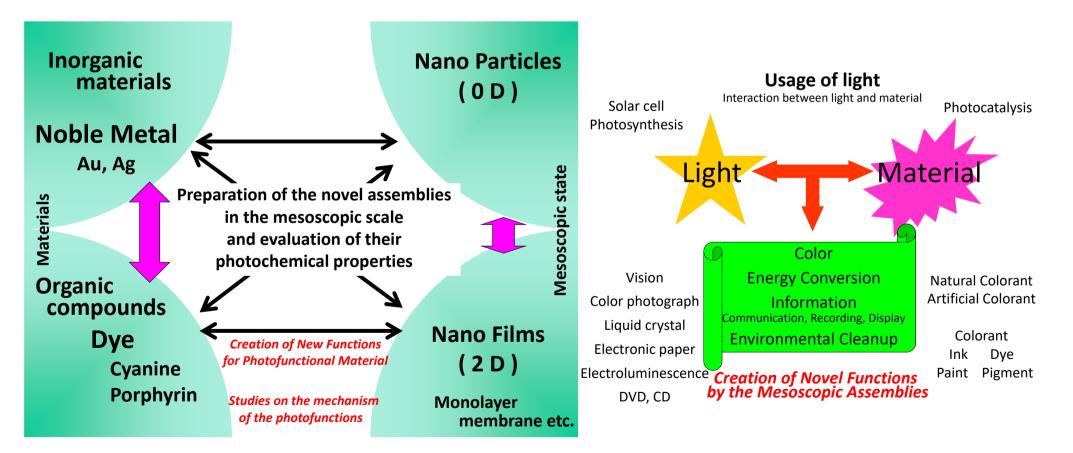


- 1) The aim is to create new urea derivatives in which the fluorescence state is changed by hydrogen bonding.
- 2) The formation and dissipation processes of fluorescent states involving hydrogen bonding with anions are analyzed kinetically by fluorescence lifetime measurements and the results are fed back to molecular design.

#### Sato Group: Tomoo SATO (Associate Professor)

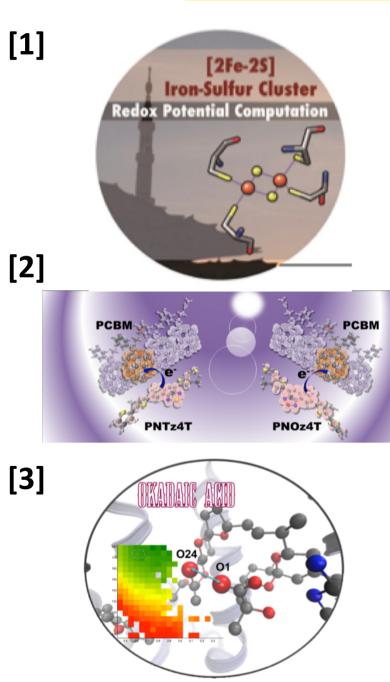
Photo physical chemistry related to surfaces, interfaces, nano-particles, and nano-films

Studies on the photofunctions and photochemical properties of the newly created assemblies in the mesoscopic scale



http://www.chem.tsukuba.ac.jp/tsato/

#### Matsui Group: Toru Matsui (Associate Professor)



### **Computational/Theoretical chemistry**

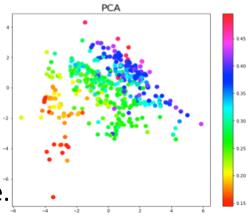
#### **Computational studies by model chemistry**

Redox potential of Fe-S model cluster [1] Rate constant for organic photovoltaics [2] Intramolecular hydrogen bonds in okadaic acid [3]

(Theme for Graduate school students) Cluster formation mechanism of citric acid Degradation mechanism of β-lactamase

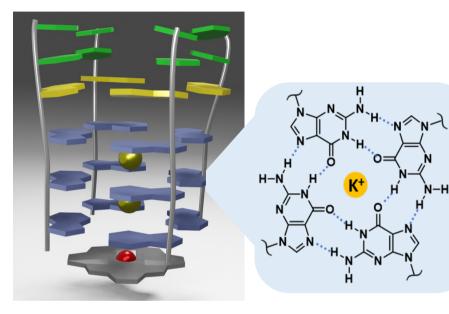
#### **Studies using machine learning (ML)**

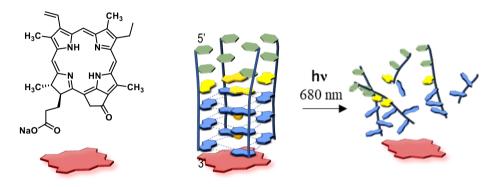
Parameters for LC-DFT Appropriate domain segmentation by reducing the dimension of the information from a molecule.



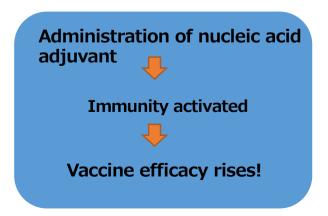
#### Momotake Group : Atsuya Momotake (Associate Professor)

- **1.** Development of highly functional and highly stable nucleic acid enzymes
- **3.** Development of photosensitizers that can be used in hypoxic regions

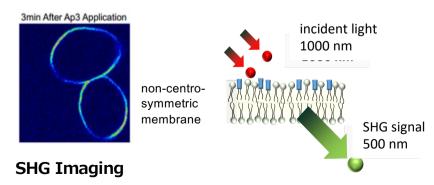




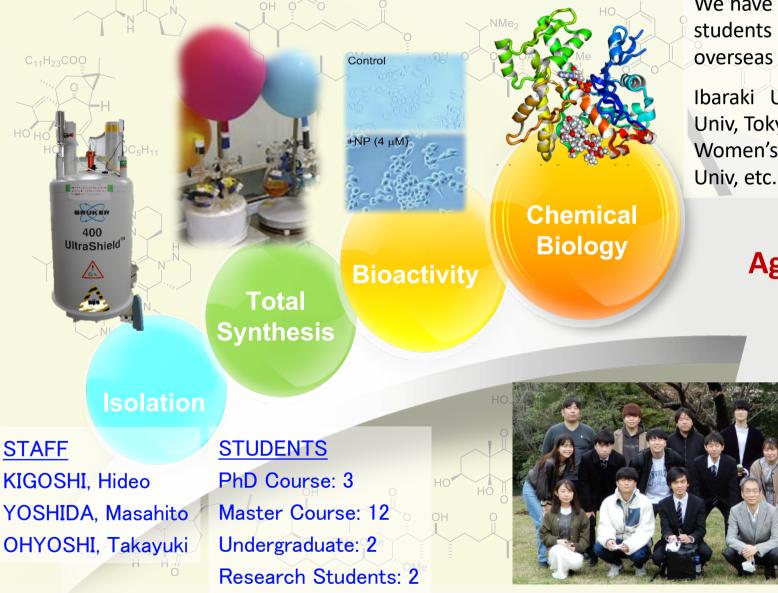
2. Development of nucleic acid adjuvants



4. Molecular Development for Nonlinear Optical Microscopy



### Bioorganic Chemistry – Natural Product Chemistry Unravel the Mysteries of Life by Organic Chemistry!



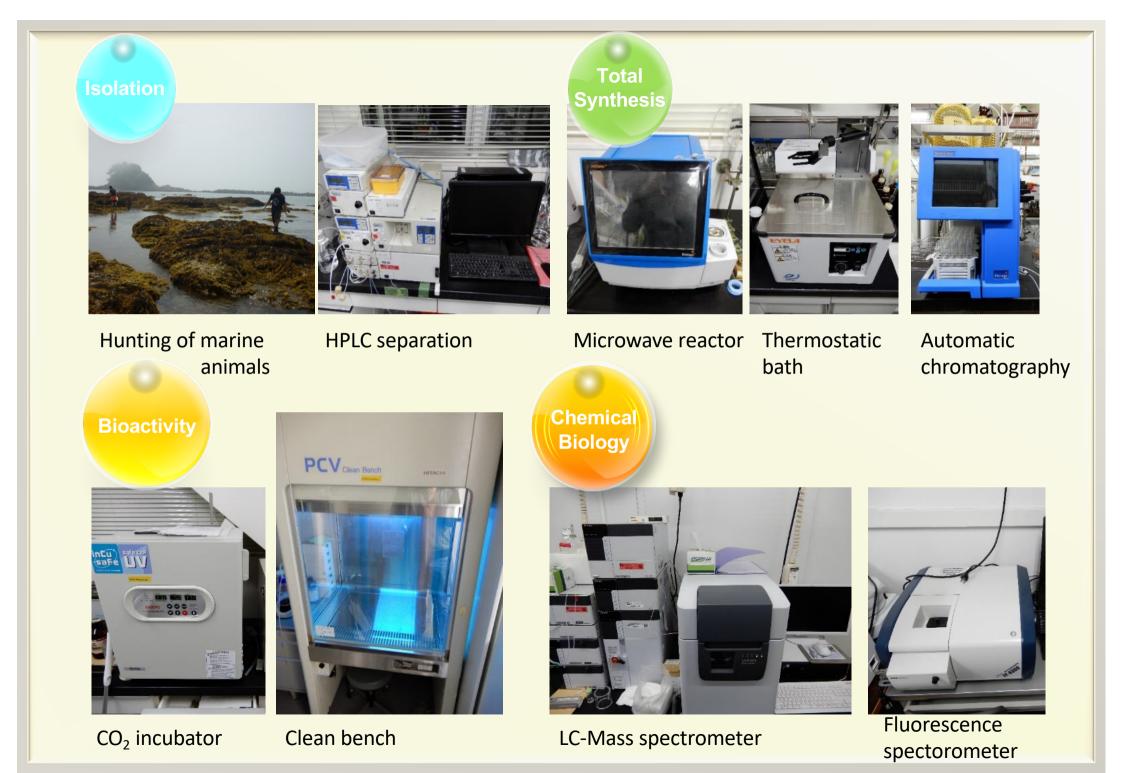
We have accepted many graduate students from domestic and overseas universities and techs:

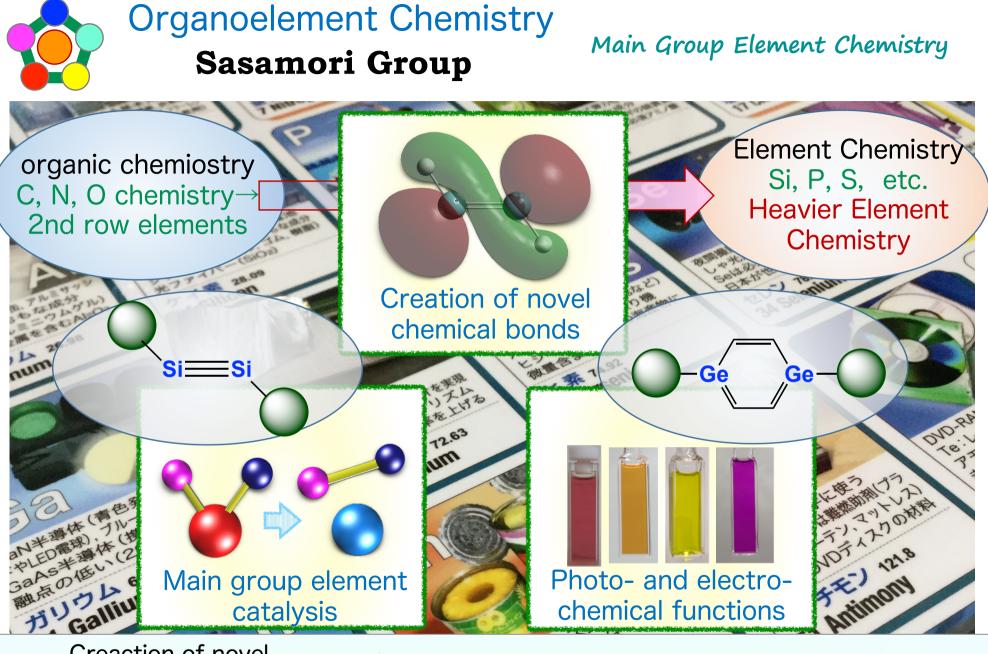
OH OH

Ibaraki Univ, Chiba Univ, Chuo Univ, Tokyo Univ of Science, Japan Women's Univ, Shanghai Normal Univ, etc.

> Medicines Agrochemicals etc.







Creaction of novel compounds utilizing specific properties of each Element

Utilizes abundant main group elements
 small molecules actibation
 novel functions



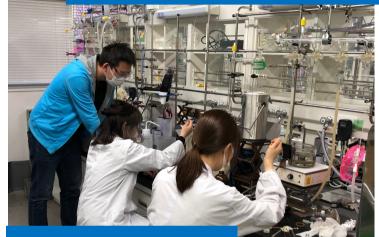
### Organoelement Chemistry Sasamori Group

BRUKER 400 UltraShield<sup>™</sup>

**NMR** 

#### Main Group Element Chemistry

Creation of Novel Compounds: custom-talored glasswares and advanced instruments



Double-manifold Ar-vacuum



Ar-column ay low-temp.



Electrochemical Measurements under Ar at L.T.



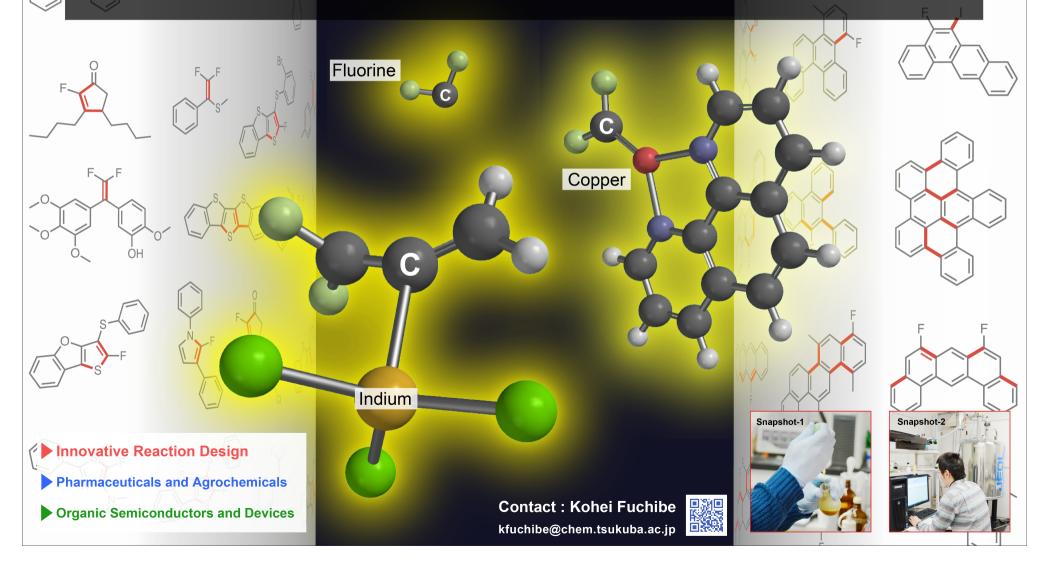
Ar glove box



Single-crystal XRD analysis

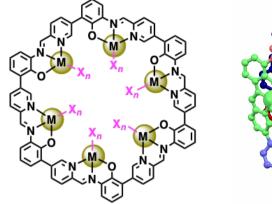
### Synthetic Organic Chemistry Powered by Novel Active Species

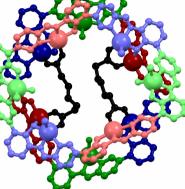
Active species are molecules and ions that promote formation of new chemical bonds, generating a wide variety of compounds. The Fuchibe Group is focusing on developing unique synthetic reactions for organic compounds by creating/utilizing characteristic active species, typically including metal elements and fluorine.



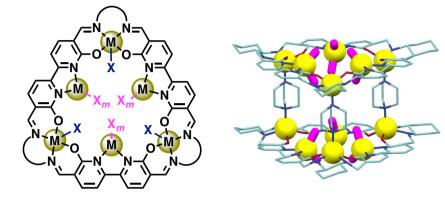
# Nakamura Group (Supramolecular Chemistry)

We design unique macrocyclic oligomers, and create supramolecules that produce novel substances through the control of functions such as molecular recognition.

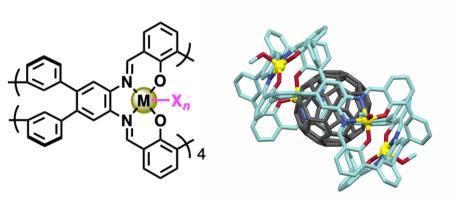


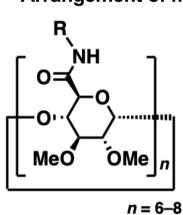


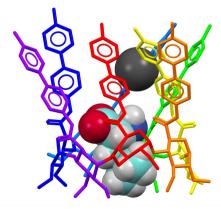
Capturing molecules by multipoint coordination



Arrangement of metal coordination sites







**Belt-shaped macrocycle** 

Amide-cyclodextrin

Nakamura group welcomes graduate students to do research together!! Contact: Takashi NAKAMURA (nakamura@chem.tsukuba.ac.jp) Web: https://www.chem.tsukuba.ac.jp/nakamura/en/index.html

# Nakamura Group (Supramolecular Chemistry)

Replace Compared Provide Analyzed Sciences University of Tsukuba Nakamura Group (Supramolecular Chemistry)

► Home	> Welcome!		
<ul> <li>Research Outline</li> </ul>	Nakamura Group (Supramolecular Chemistry), University of Tsukuba. We design and synthesize unique macrocyclic oligomers, and create supramolecules that produce novel		
<ul> <li>Members</li> </ul>	substances through the control of functions such as molecular recognition.		
<ul> <li>Publications</li> </ul>	Y News		
<ul> <li>Research Facilities</li> </ul>	Apr. 08, 2022	Assist. Prof. Nakamura receives the Young Scientist's Award in the Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, Japan ( <u>MEXT webpage (Japanese</u> )). <b>NEW</b>	
<ul> <li>Contact / Access</li> </ul>	Apr. 05, 2022	Members and Photo Gallery have been updated. NEW	
► Photo Gallery	Mar. 04, 2022	Our introduction video has been uploaded to YouTube.	
	o Jan. 20, 2022	Assist. Prof. Nakamura has been awarded as 2021 BEST FACULTY MEMBER, University of Tsukuba.	
► Link	Y Admission	S	



Nakamura group welcomes graduate students to do research together!! <u>Master's/Doctoral Program in Chemistry</u> <u>Master's/Doctoral Program in Materials Innovation</u>

#### Introduction Video (March 2022)



Our research group has started since April 2021.

Let's experience the fun of research and build up a new chemistry!!

Nakamura group welcomes graduate students to do research together!! Contact: Takashi NAKAMURA (nakamura@chem.tsukuba.ac.jp) Web: https://www.chem.tsukuba.ac.jp/nakamura/en/index.html

### Iwasaki's Laboratory Structural Biology and Chemistry

Elucidate the structure of biomolecules to unravel the mysteries of life, elucidate pathogenesis at the molecular level, and help in the latest drug discovery (not only small molecule drugs, but also middlemolecule drugs, the latest technology in biomolecular drugs, and gene therapy). One billion yen national project Two of the cutting edge cryo-electron microscopes for drug discovery was installed in our laboratory in FY2021.

創薬研究に産学連携拠点 筑波大

クライオ電子顕微鏡お披露日

Elucidating Pathogenesis at the Molecular and Atomic Levels Contributing to Drug Discovery for Therapy



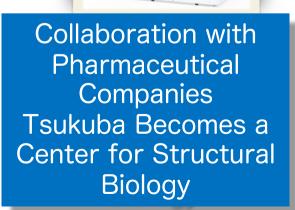
The cryo-EM image gives us the atomic coordinates of the molecule!

(a technique that won the 2017 Nobel Prize in Chemistry)

Elucidating the Molecular Mechanism of Synovial Sarcoma Development

Elucidation of the Molecular Mechanism of Malignant

- Lobular Tumor Development
- Elucidation of the Mechanism
   of Optical Sensor of *Euglena*



Cryo-EM

E.S.

# cryo-EM@Univ. of Tsukuba

The cryo-electron microscopes are in the P2 room.

CRYO-ARM 300II

CRYO-ARM 200

### JEM-1400+TVIPS 4K Elsa holder







Prof. : Noriki Kutsumura Assistant Prof. : Tsuyoshi Saito Uur group is located at the IIIS building. This research organization is home to world-class specialists in brain research and sleep research, who work hard every day to conduct research that transcends the boundaries between laboratories. We are the only **chemistry group** in IIIS. We are engaged in various collaborative research projects using **drug discovery technologies based on synthetic organic chemistry**. We are also collaborating with many pharmaceutical companies and have some drugs under clinical trials.





睡眠医科学研究棟



研究室内の様子



濃縮



マウスに化合物を投与



抽出



化合物の質量測定





研究室内の様子



化合物を細胞で評価中



濾過

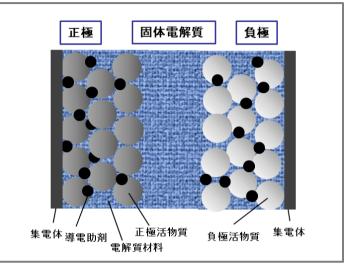
### Cooperative Graduate School System (AIST Tsukuba Central)

Research Field	Professor	Research
Material Inorganic Chemistry	Junji AKIMOTO	Studies on inorganic solid state chemistry and electrochemistry for advanced functional materials (including lithium ion battery positive and negative electrode materials, and advanced solid electrolyte materials).
Surface Electrochemistry	Yukari SATO	Functionalization of solid and electrode surfaces; Redox flow battery for renewable energy introduction; Construction of micro multi sensing devices for marine environment.
High-pressure Organic Chemistry	Hajime KAWANAMI	Research on various organic chemistry with a ley word of "high-pressure".
Organic Electronics Chemistry	Yuji YOSHIDA	Research on structural properties and photo-electrical properties of thin films based on polymers, molecular compounds and organic-inorganic hybrid materials, and chemistry on organic electronics such as organic photovoltaic cells (solar cells).
Nano-carbon Materials Chemistry	Toshiya OKAZAKI	Synthesis of the functionalized nano-carbons and their spectroscopic characterizations.
Organometallic Chemistry	Yumiko NAKAJIMA	Chemistry Design and synthesis of novel transition metal catalysts, development of catalytic reactions for precise synthesis of new organometallic compounds containing main group elements.
Photofunctional Material Chemistry	Yasuo NORIKANE	Photofunctional organic molecules especially showing photo-induced solid- liquid phase transitions and light-driven mechanical motion.
Functional Polymer Gel Chemistry	Yusuke HARA	Research and development of functional polymers and polymer gels for application to soft actuators, soft robots, micro fluidic devices.

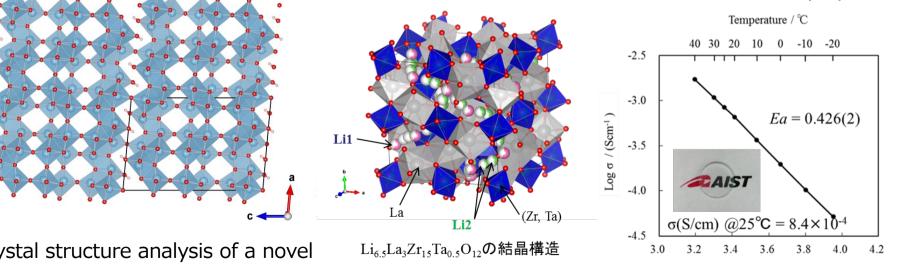
#### Materials Inorganic Chemistry Lab. Prof. Junji Akimoto (j.akimoto@aist.go.jp) in AIST

Research Title: Study on Inorganic Oxide Materials for High Performance Battery Applications

Lithium-ion batteries are expected to be widely used and deployed in large-scale applications such as electric vehicles (EV) and stationary power supplies. In order to realize next-generation high performance battery system, we are studying on new oxide materials utilizing by single crystal growth technology, soft chemical synthesis method, flux synthesis method, hydrothermal synthesis method, etc. In addition, we are studying on new material design by applying accurate crystal structure analysis and electrochemical and physical property measurements for inorganic compounds.



All Solid-State Battery System



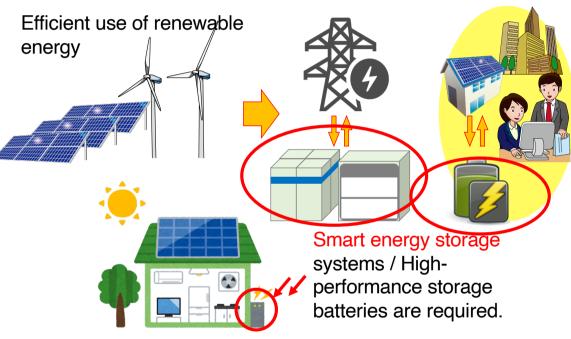
1000 / T (K<sup>-1</sup>)

Crystal structure analysis of a novel titanium oxide prepared by soft-chemical synthesis.

Crystal structure analysis and electrochemical measurements of garnet-type lithium-ion conducting oxide.

#### 連携大学院表面電気化学研究室(佐藤 緑 @ 産総研) Surface Electrochemistry Lab. (yukari Sato @ AIST)

### **Redox Flow Batteries**



#### Contact:

Yukari SATO <u>yukari-sato@aist.go.jp</u> Central 5, 1-1-1 Higashi, Tsukuba, AIST 産総研つくば中央第5内 見学は随時可能です! https://unit.aist.go.jp/ieco/groups/index.html#esg https://unit.aist.go.jp/ieco/est-2021/ We are conducting research and development of new RFBs that are no resource constraints and have low environmental impact.





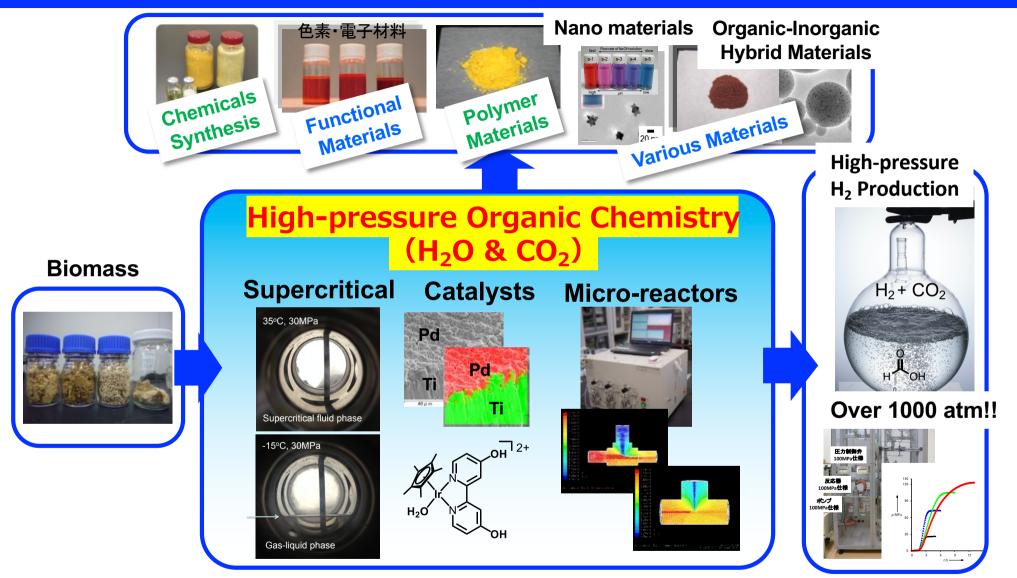
Environmental protection: Continuous measurement of Sea water pH



In order to predict environmental changes, we will make a small measuring device and observe pH changes. Joint research with the U. of Tokyo. 海水のpH連続測定、東大理と共同研究、

#### High-pressure Organic Chemistry Lab., Prof. Hajime Kawanami@AIST

h-kawanami@aist.go.jp, https://irc3.aist.go.jp/incorporate/team/functional-transformation/

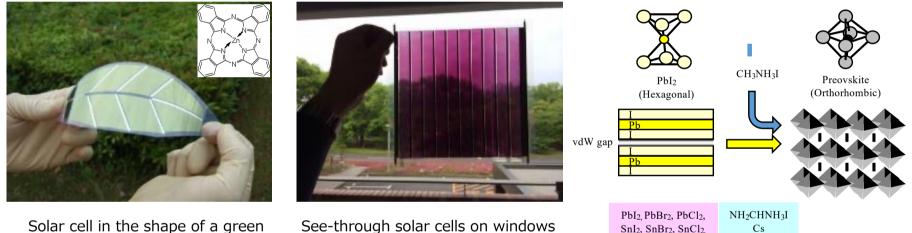


We are focusing on organic chemistry using high-pressure such as supercritical fluids. Recent topics are high-pressure H<sub>2</sub> productions over 100 MPa from formic acid, and biodegradable polymer syntheses from biomass.



#### Organic Electronics Chemistry Laboratory, Cooperative Graduate School (AIST) Professor Yuji YOSHIDA

Our research aim is to solve the world's  $CO_2$  reduction and energy problems with light and flexible solar cells. With conducting polymers (polythiophene), molecular dyes (phthalocyanine), and inorganic semiconductors (perovskite compounds) that can be painted, we are creating new concepts of solar cells with excellent design that can be installed on windows and walls or mounted on mobility vehicles.



Solar cell in the shape of a green leaf using phthalocyanine

See-through solar cells on windows

Effect of passivation on the interface between perovskite and donor-acceptor copolymer-based holetransport layer in perovskite solar cells, Chem. Lett., 49, 1341, 2020

Investigation of the electron transport layer in semitransparent organic photovoltaic cells using near-infrared light-absorbing materials J.pn J. Appl. Phys., 60, 071004-1-6, 2021

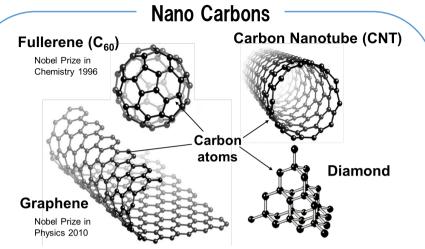
Organic-inorganic hybrid perovskite crystal structure that can be solution coated (power conversion efficiency is comparable to silicon)

(Ge, Bi, ...)

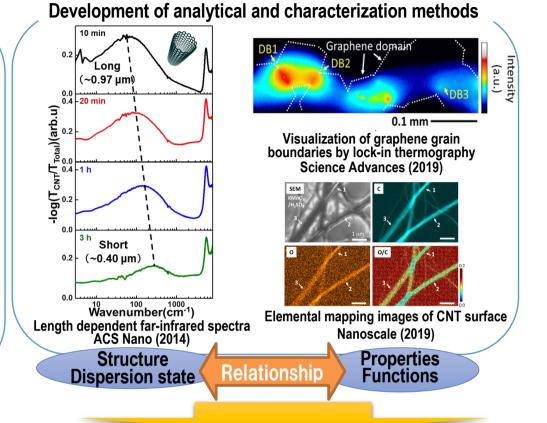
#### Yoshida's Lab.

Cooperated with organic-inorganic hybrid PV team, Global zero emission research center, AIST [Contact address]E-mail: yuji.yoshida@aist.go.jp / URL: https://staff.aist.go.jp/yuji.yoshida/

#### Cooperative Graduate School (AIST) Toshiya Okazaki's lab (Associate Professor)



- Light weight and mechanically strong
- Chemically stable
- Electrically and thermally conductive
- Nano scale in size and high specific surface area

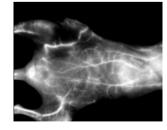




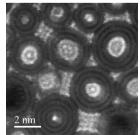
2020 Lab Members

Nano Carbon Device Research Center, AIST





NIR imaging probe Sci Rep (2014)



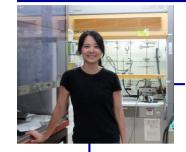




**CNT liquid crystal** 

E-mail: toshi.okazaki@aist.go.jp

#### Organometallic Chemistry Laboratory\_ Cooperative Graduate School Dr. NAKAJIMA, Yumiko@AIST



Development of New Catalytic Reactions towards Development of High-Performance Materials

Organometallic Catalysts

Synthetic Chemistry Labworks







Theoretical Calculations

Efficient synthesis of highperformance materials





Fiber-reinforced Eco-tire plastic

Encapsulant of devices

etc

Analysis Using High-Performance Equipments



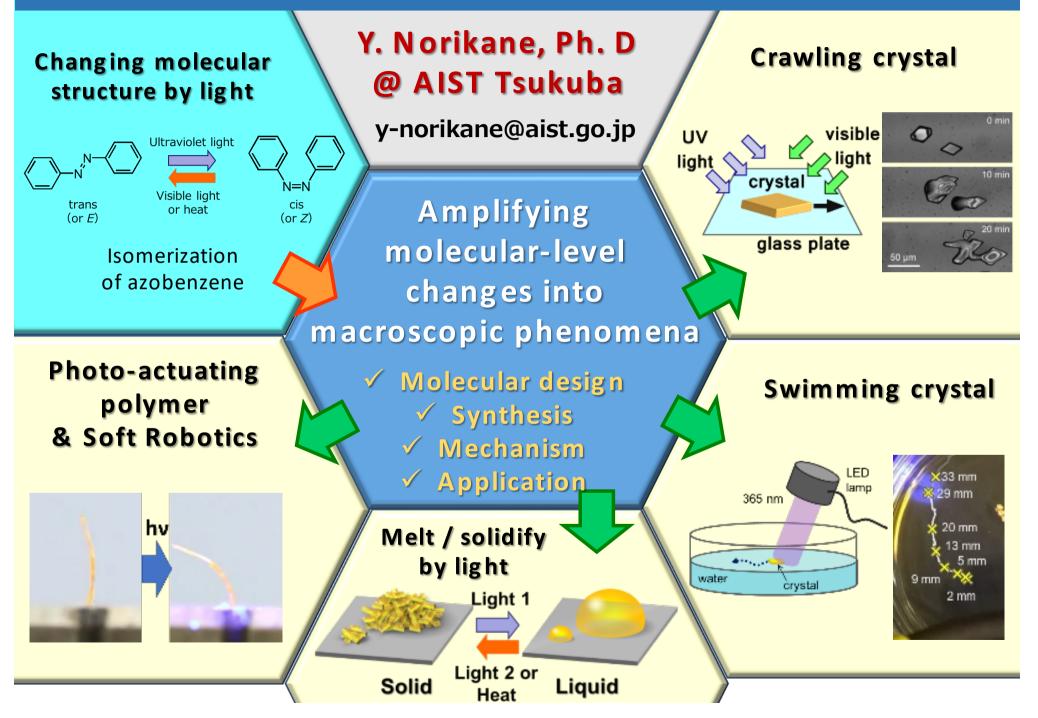


Financial supports are available

¥200,000 JPY/month for Doctor course students ¥100,000 JPY/month for Master cource students

(contact) yumiko-nakajima@aist.go.jp, URL: http://irc3.aist.go.jp/team/organosilicon-chemistry/

### **Photofunctional Materials Lab.**



### **Functional Soft Material Laboratory**

Associate professor Yusuke Hara



#### Study on Soft Actuators

Development of soft actuators in microchannels driven by chemical reactions, electric field, pH, etc.

Study on Capillary Gel Electrophoresis

Development of novel gels that can accurately, quickly, and easily separate DNA fragments.

Study on process informatics by machine learning

By applying machine learning to flow synthesis, we improve and optimize the process of the flow synthesis method.

Degree Programs in Pure and Applied Sciences, Graduate School of Science and Technology, University of Tsukuba

Master's/Doctoral Program in Chemistry

https://program.chem.tsukuba.ac.jp/



