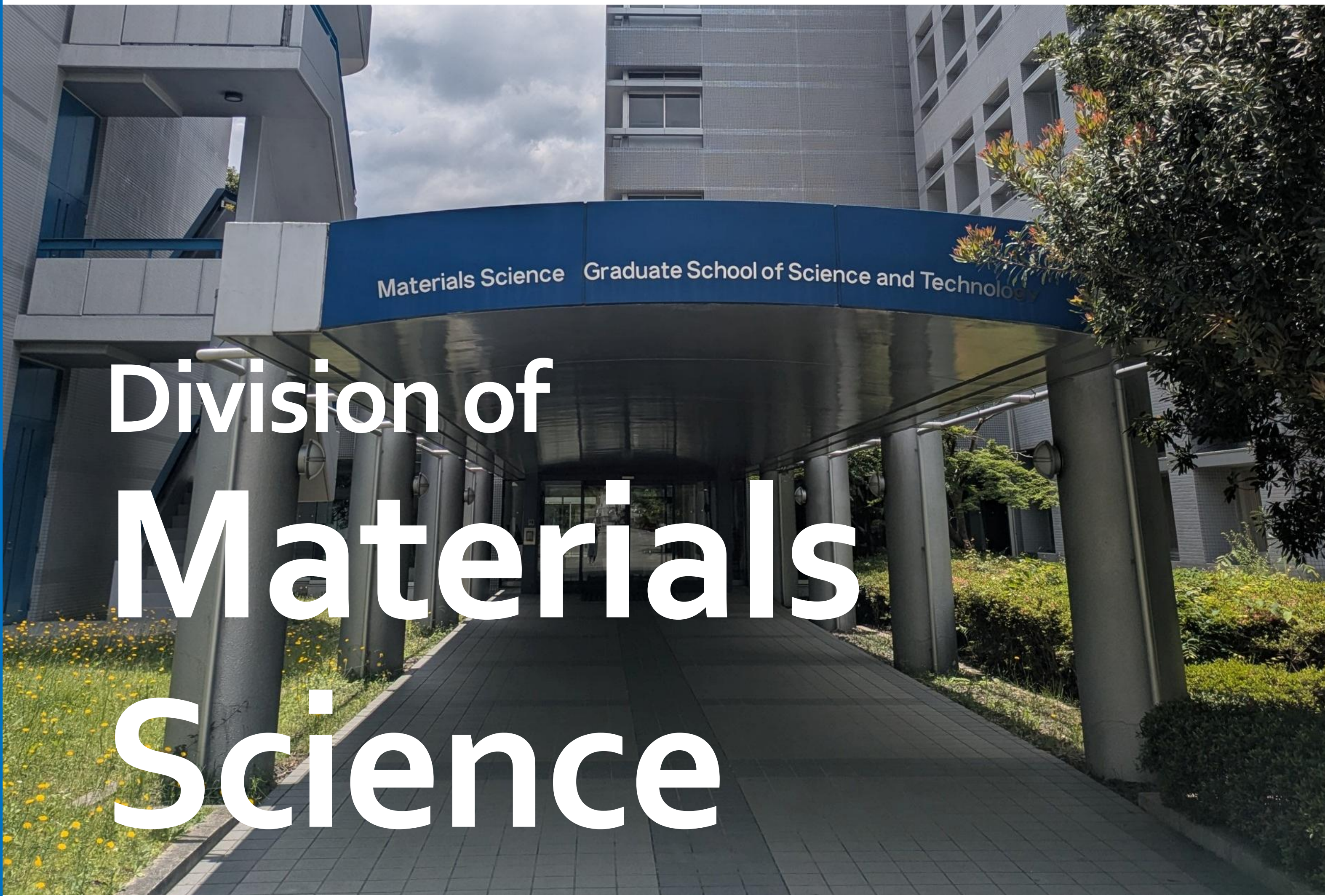
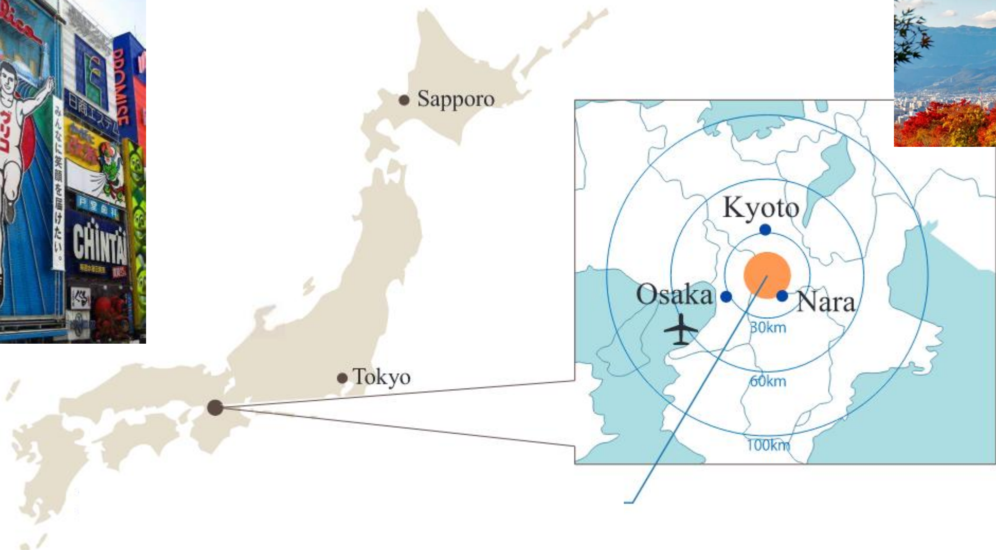


Division of Materials Science

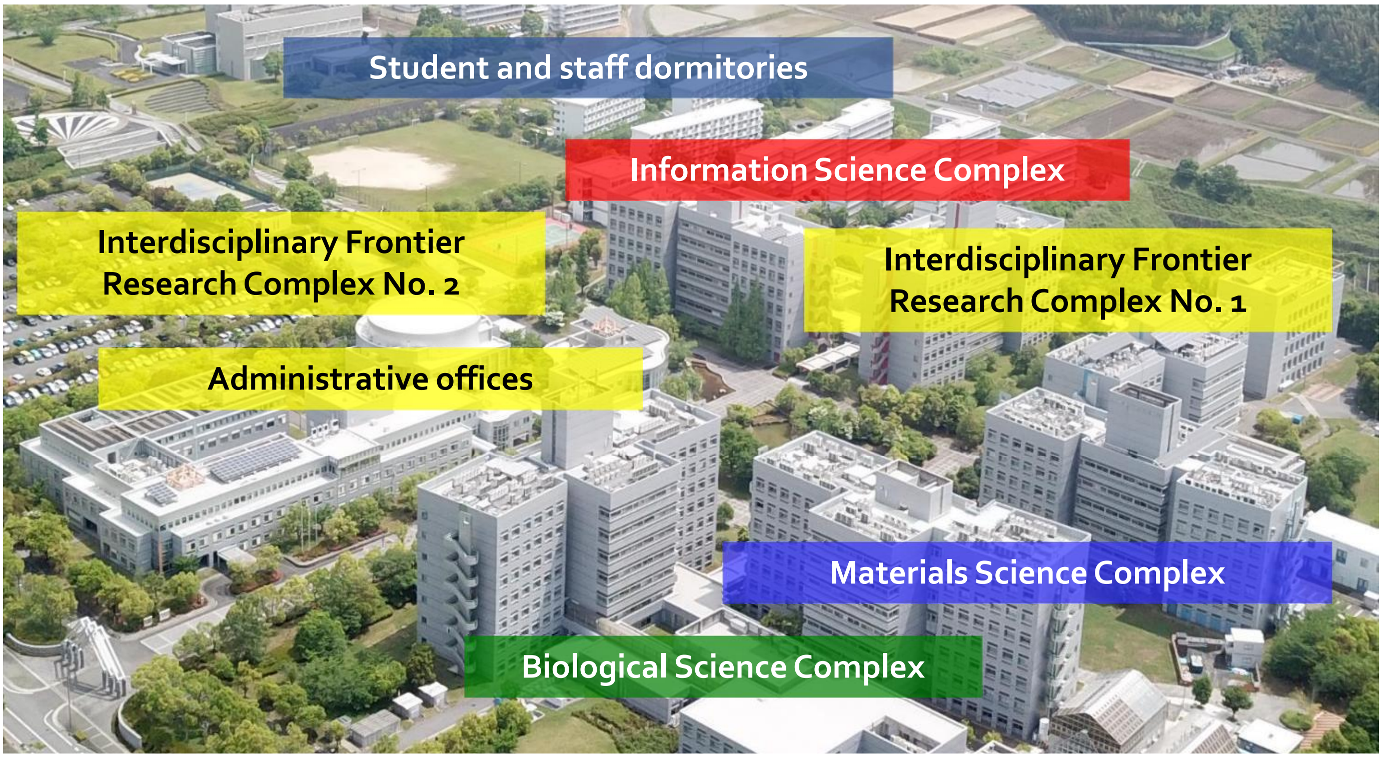
Nara Institute of Science and Technology

Location and Campus

NAIST is located in Nara Prefecture. Home of the first official capital of Japan, Nara Prefecture has an incredibly rich history as a center for international trade and relations. It is also conveniently located in close proximity to Kyoto and Osaka.



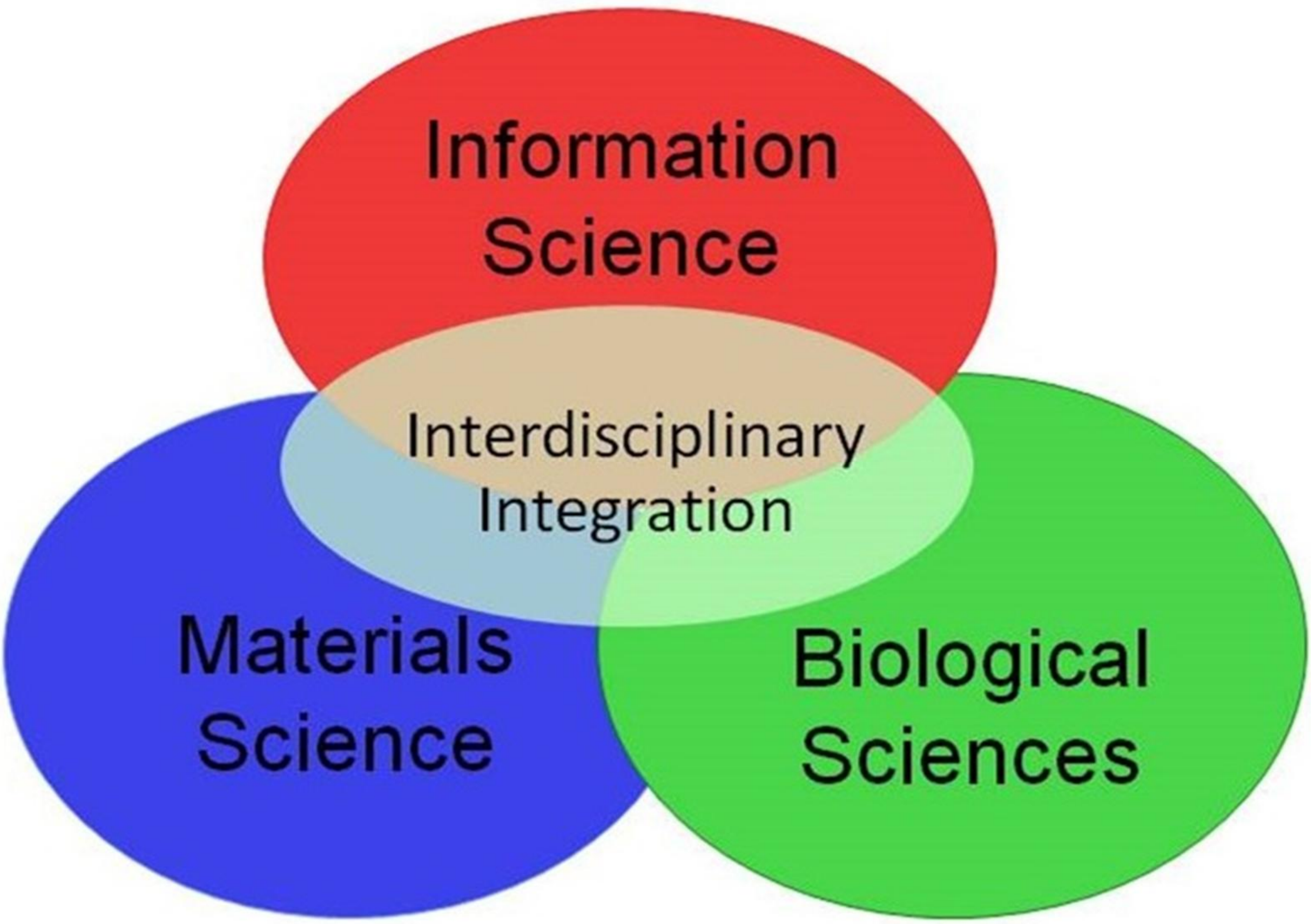
Kansai Science City, a research park located in a area stretching over Kyoto, Osaka, and Nara prefectures. The area of the city is 150 km², with more than 150 research facilities, universities, and cultural facilities.



NAIST occupies 137 thousand square meters of land, or approximately 14 hectare.
So NAIST is a very compact university. And In the division of Materials Science, we have 274 students, including 57 international students from 13countries. It's almost 20% are from abroad.

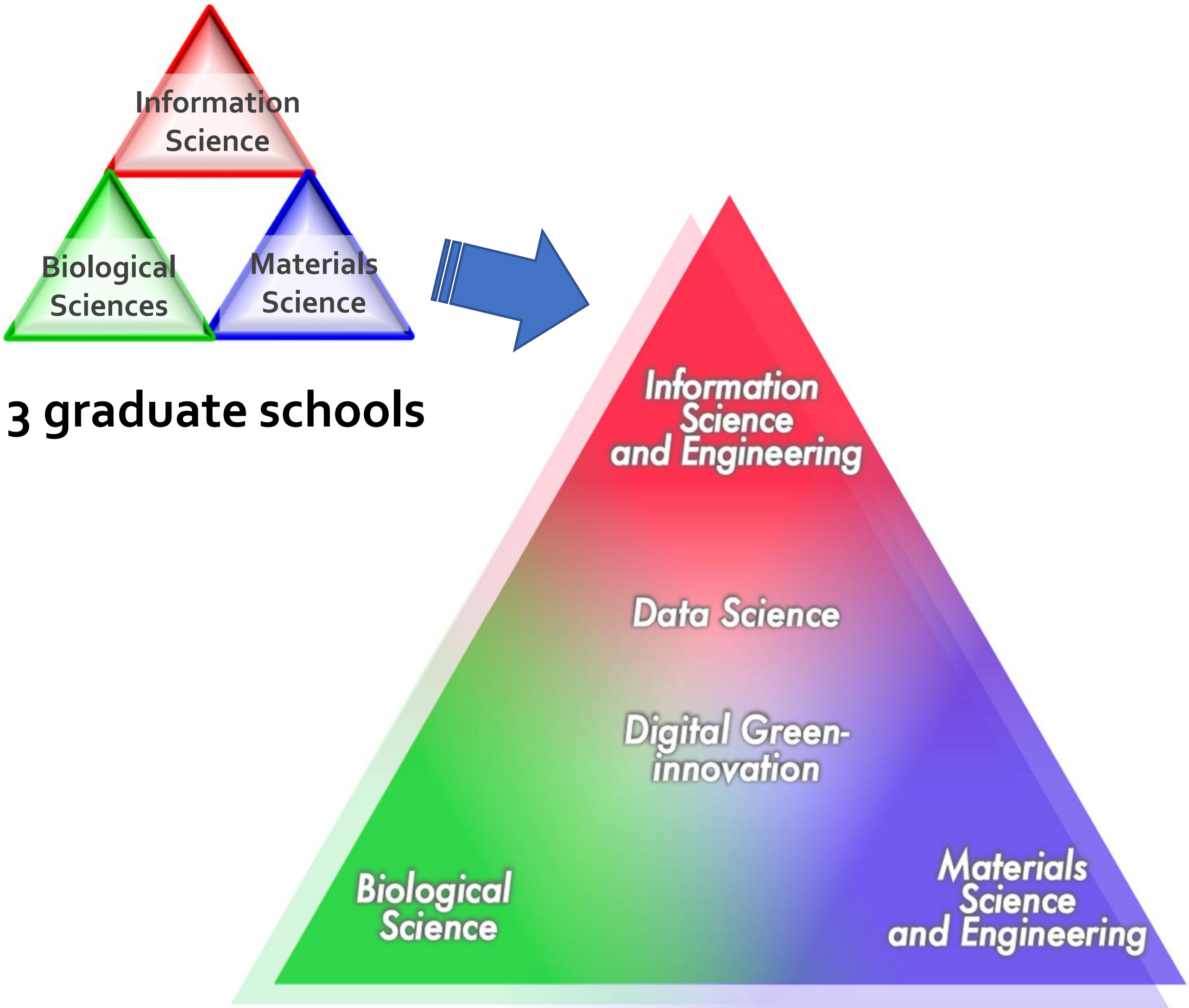
Science and Technology

Founded in 1991 as a unique national university, NAIST was composed solely of graduate schools, and had been focused on three priority areas and their fusion domains of science and technologies.



One graduate school

Founded in 1991 as a unique national university, NAIST was composed solely of graduate schools, and had been focused on three priority areas and their fusion domains of science and technologies.



Graduate School of Science and Technology With five educational programs

In April, 2018, NAIST underwent an organizational transformation to lower barriers between academic fields and become a single graduate school with seven education programs. NAIST evolved again in April, 2022, and merged the seven programs into five. The new Graduate School of Science and Technology allows NAIST to further adapt to the ever-changing needs of society and developments in science and technology.

Message from the Director

Welcome to the website of the Division of Materials Science at Nara Institute of Science and Technology (NAIST).

Our Division has a distinguished 25-year history, originating from the Graduate School of Materials Science. Over the years, we have consistently achieved world-leading research outcomes across diverse fields, including physics, device engineering, chemistry, biomaterials, data-driven science, and beyond.

With state-of-the-art facilities and the dedicated expertise of our research staff, we are committed to further advancing cutting-edge research. Our focus includes exploring novel quantum phenomena, developing innovative devices, pioneering next-generation measurement and process technologies, and creating groundbreaking new compounds, polymers, and protein materials. Moreover, we are dedicated to ensuring that these achievements benefit society.

Building upon this strong foundation, NAIST has been selected for the J-PEAKS program, marking our transition into a leading graduate research university. As part of university-wide initiatives, the Division of Materials Science will play a crucial role in driving the digitalization of materials science research, integrating both experimental ("hardware") and analytical ("software") aspects. We are also eager to take on even greater challenges in both research and education. As we embark on this transformative journey as a new graduate university, I am deeply aware of my responsibility as Director of this Division and excited about the opportunities ahead.

NAIST has a long-standing commitment to internationalization, warmly welcoming students from around the world. We provide a comprehensive career support system, including programs that connect students with Japanese companies during their studies. As a result, approximately 30% of our international graduates have successfully secured positions in Japanese private companies. Through the J-PEAKS initiative, we aim to strengthen collaborations with international universities, significantly expanding joint and double-degree programs. The active participation of international students and researchers is essential for the continued growth of both NAIST and our Division of Materials Science.

By uniting our efforts with faculty, staff, and students, as well as domestic and international companies and external organizations that share our vision, we will continue to push the frontiers of materials science and its interdisciplinary fields. At the same time, we remain dedicated to cultivating highly specialized researchers and experts who will shape the future, fostering an environment where knowledge and technology are effectively translated for societal benefit.

We sincerely appreciate your continued interest in the Division of Materials Science and warmly invite you to join us in shaping the future.

Hironari KAMIKUBO,
Director,
Division of Materials Science

Research Units (Laboratories)

in 2025

- ◆ 16 Core Laboratories
- ◆ 2 Core Laboratories (Cooperative)
- ◆ 5 Core Laboratories (Collaborative)
- ◆ 1 Affiliate Laboratory

Physics

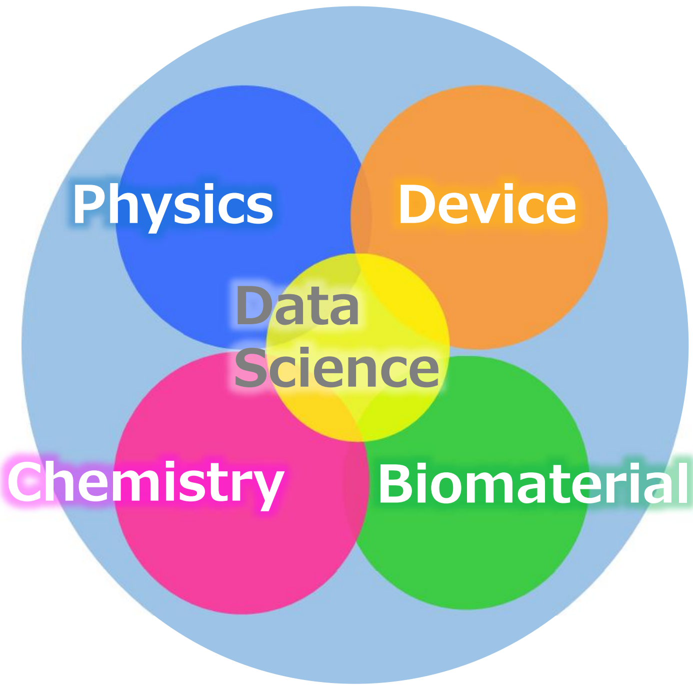
- ◆ Bio-Process Engineering
- ◆ Solid-state Information Physics
- ◆ Quantum Photo-science

Device

- ◆ Information Device Science
- ◆ Applied Quantum Physics
- ◆ Organic Electronics
- ◆ Photonic Device Science
- NEW Thin Film semiconductor Devices
- ◆ Mesoscopic Materials Science (Panasonic)
- ◆ Sensory Materials and Devices (Shimadzu)

Chemistry

- ◆ Photonic and Reactive Molecular Science
- ◆ Biomimetic and Technomimetic Molecular Science
- ◆ Functional Organic Chemistry
- NEW Functional Inorganic Materials Design*
- ◆ Functional Polymer Science (Santen)
- ◆ Ecomaterial Science (RITE)
- ◆ Advanced Functional Materials (OMTRI)
- ◆ Interfaces, Molecules and Materials



Data Science

- ◆ Materials Informatics
- ◆ Data Driven Chemistry
- ◆ Metrology Informatics

Biomaterial

- ◆ Functional Supramolecular Chemistry
- ◆ Complex Molecular Systems
- ◆ Nanomaterials and Polymer Chemistry

Bio-Process Engineering

Education and Research Activities

The Bio-Process Engineering Laboratory promotes developmental research of high-precision and fast manipulation methodologies for small biological materials, utilizing ultra-short pulse laser technology. When an intense femtosecond laser is focused in the vicinity of a micro-sized biological micro-object in a water medium, an explosion of water is induced at the laser focal point, and shock and stress waves from the explosion act as an impulsive force on the sample (Fig. 1). We have developed several methodologies to manipulate single animal and plant cells utilizing this impulsive force. In addition, this laser manipulation technology has been combined with atomic force microscopes (AFM), microfluidic chip devices, and spectroscopy devices. The AFM is applied to quantify impulsive force and to analyze the sample oscillation induced by that force (Fig. 2). Microfluidic chip devices fabricated by MEMS technology realize sequential high-speed laser manipulation and measuring of biological micro-objects (Fig. 3). Spectroscopy devices are used to identify characteristics of objects manipulated by laser and/or microfluidic chip. Using these techniques, we successfully estimated the adhesion strength between mammalian cells and between sub-organelles in plant cells. Furthermore, we apply such femtosecond laser-induced strong excitation phenomena to photoporation for living vertebrate embryos and alga (Fig. 4) and to induce crystallization (Fig. 5). In an application of microfluidic chip-based cell sorter, we successfully manipulated cells at 100,000/s (World Class). These activities and devices aim to open up entirely new areas of life and green innovation. The laboratory fosters human resources with a broad knowledge of engineering and science from areas ranging from physics and chemistry to biology and medicine. Laboratory members are ambitious to pursue a blazing trail in life science and engineering fields.

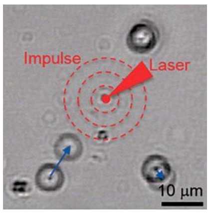


Fig.1 Manipulation of micro-beads by femtosecond laser impulse

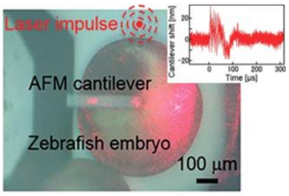


Fig.2 Nanometer scale vibration of Zebrafish embryo induced by laser impulse and detected by AFM

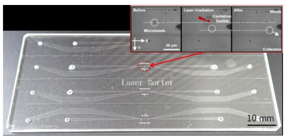


Fig.3 High-speed laser manipulation in micro-fluidic chips

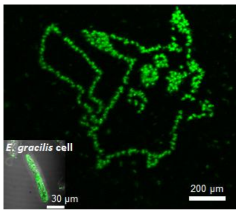


Fig.4 Laser scanning photoporation of fluoresce probe molecules at single cell resolution

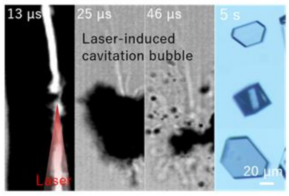


Fig.5 High-speed observation of anthracene crystallization triggered by a ultrashort laser pulse

Research Theme

1.Kinetics of local explosions in water induced by ultrashort laser pulses, and its interaction with biological micro-objects
2.Development of new measurement methods to estimate internal stress in living tissues utilizing ultrashort lasers and atomic force microscopes
3.Development of new cell manipulation techniques in microfluidic chips
4.Exploration of the responsiveness of cells and living tissues to the environment stress and its application to cell manipulation

Staff and Contact

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Recent Research Papers and Achievements

1. Y.Hosokawa, M.Hagiyama, T.Iino, Y.Murakami, A.Ito, “Noncontact estimation of intercellular breaking force using a femto-second laser impulse quantified by atomic force microscopy,” Proc. Nat’l Acad. Sci. USA, 2011, 108, 1777-1782.
2. K.Oikawa, S.Matsunaga, S.Mano, M.Kondo, K.Yamada, M.Hayashi, T.Kagawa, A.Kadota, W.Sakamoto, S.Higashi, M.Watanabe, T.Mitsui, A.Shigemasa, T.Iino, Y.Hosokawa, M.Nishimura, “Physical interaction between peroxisomes and chloro plasts elucidated by in situ laser analysis,” Nature Plants, 2015, 1, 15035.
3.Y.Hosokawa, H.Ochi, T.Iino, A Hiraoka, M.Tanaka, “Photoporation of biomolecules into single cells in living vertebrate embryos induced by a femtosecond laser amplifier,” PLoS ONE, 2011, 6, e27677.
4.T.Maeno, T.Uzawa, I.Kono, K.Okano, T.Iino, K.Fukita, Y.Oshikawa, T.Ogawa, O.Iwata, T.Ito, K.Suzuki, K.Goda, Y.Hosokawa, “Targeted delivery of fluorogenic peptide aptamers into live microalgae by femtosecond laser photoporation at single-cell resolution,” Sci. Rep., 2018, 8, 8271.
5.T.Iino, K.Okano, S.W.Lee, T.Yamakawa, H.Hagihara, Z.Y.Hong, T.Maeno, Y.Kasai, S.Sakuma, T.Hayakawa, F.Arai, Y.Ozeki, K.Godab, and Y.Hosokawa, “High-speed microparticle isolation unlimited by Poisson statistics,” Lab Chip, 2019,19, 2669- 2677.

Solid-State Information Physics

Education and Research Activities

1. Research purpose and target

Functional materials are created by adding dopant atoms to the material or depositing atoms on the surface. The added atoms in bulk work as active sites and dramatically change the material's properties. Also slightly deposited atoms on surfaces can change structures and functionalities. Visualizing the three-dimensional atomic arrangement and understanding the function generation mechanism will bring about technological innovation. Our laboratory is the first in the world to develop photoelectron holography (PEH) to visualize dopant sites, and in developing apparatus in SPring-8. Our laboratory also studies surface structures, electronic states, and magnetism using scanning tunneling microscopy (STM), reflection high-energy electron diffraction (RHEED), low-energy electron diffraction (LEED), angle-resolved photoelectron spectroscopy (ARPES), cathode luminescence (CL), etc. For data science, we use a combination of scattering quantum mechanics, density functional theory (DFT), and artificial intelligence (AI). Our research targets include semiconductors, oxides, and alloys; atomically-controlled surfaces and nano-films/wires/dots, artificially designed 3D shaped structures, and nano-scale space charge layers. Our aim is to clarify the physical properties of active sites and modified surfaces, while creating new functions from atomic and electron viewpoints.

2. Educational policy

We provide education on experiments and physics combined with informatics. Also, we aim to develop important skills for researchers and professional engineers, which include an active attitude toward obtaining knowledge through acquisition of technical expertise (such as shop practices, machine control, and data analysis), cooperation with laboratory members, finding essential points based on logical thinking, presenting ideas, and managing activities. Students are expected to improve or create apparatuses before graduation. It is important for students to not only learn how to think systematically through seminars and lectures, but also to interact with external researchers in addition to the regular laboratory educational staff.

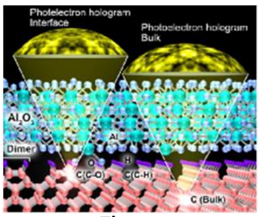

Fig. 1

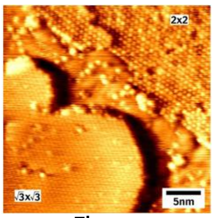

Fig. 2

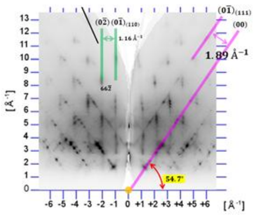

Fig. 3

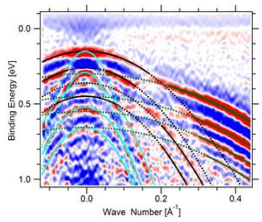

Fig. 4

Fig. 1 Photoelectron holography
Fig. 2 Atomic-scale STM image of ultra-thin film and island of iron-silicides on a Si(111) surface.
Fig. 3 3D-RSM of a 3D elongated island of α-$FeSi_2$(110) on Si(001).
Fig. 4 Si valence subbands in p-type inversion layer.

Research Theme

1. Atomic structural analysis of active sites in/on materials by PEH
2. Quantum theory of scattering combined with AI
3. Creation of 3D Si structures with nano-films using lithography, STM, LEED, RHEED
4. Surface roughness analysis by RHEED
5. Electronic states of 3D-Si structures and semiconductor space charge layers by ARPES and AI
6. Surface defects by surface sensitive CL

Staff and Contact

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Recent Research Papers and Achievements

1. Y. Li, Y. Hashimoto, T. Matsushita et al., Sci. Rep., 15, 8366 (2025).
2. M. N. Fujii, Y. Hashimoto, T. Matsushita et al., Nano Lett. 23, 1189 (2023).
3. T. Yokoya, T. Matsushita, et al., Nano Lett. 19, 5915 (2019).
4. H. Tanaka, K. Kuroda, T. Matsushita, J. Elec. Spec. Rel. Phenom. 264, 147927 (2023).
5. A. Irmikimov, K. Hattori, et al., ACS Cryst. Growth Des. 21, 946 (2021).
6. K. Hattori, Y. Sakai, L. N. Pamasi, et al., eJSSNT 20, 214 (2022).
7. N. I. Ayob, T. J. Inagaki, H. Daimon, S. N. Takeda, Jpn. Appl. Phys. 60, 064004-1 (2021).

Quantum Photo-Science

Education and Research Activities

The Quantum Photo-Science Laboratory studies various types of quantum states of target systems by using shaped ultrashort laser pulses and nonlinear spectroscopic techniques.
While most properties of material are determined by the characteristics of constituent atoms and molecules, sometimes new and exotic optical and electromagnetic properties may appear in the coherent state, in which many atoms and molecules share a common phase factor. In our laboratory, we are interested in the quantum mechanical properties of materials, including the microcavity polaritons, coherent phonons, and two-dimensional semiconductor materials. We utilize lasers to investigate the ultrafast dynamics of such systems, looking for the applications such as polariton-based catalysis for chemical reactions, light emitting devices and photo-switching devices.

Research Theme

1. Ultrafast dynamics of vibrational polaritons

Vibrational polariton is a mixed quasiparticle of Mid-IR photon and molecular vibrational motion. Recently, it is shown that the formation of vibrational polariton can affect various properties of molecules. We apply ultrafast spectroscopic techniques to reveal the background physics and chemistry of such new phenomena.

2. Coherent control of condensed phase quantum states

Coherent control is a technique to manipulate the quantum wavefunction of target systems by precisely designed laser pulses. We apply this technique to control the coherent phonon motion in various single crystalline systems. Our goal is to trigger a photo-induced phase transition induced by electron-phonon interactions.

3. two-dimensional semiconductor for nano-photonic devices

Transition metal dichalcogenide is a two-dimensional material with a finite bandgap. Depending on the number of layers, its optical properties change drastically. In particular, monolayer TMDC is promising for optoelectronic applications due to its high emissivity. We combine TMDC with our microcavity environment to develop room temperature quantum devices.

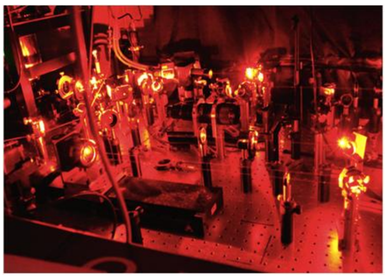

Fig. 1 Experimental setup for ultrafast nonlinear spectroscopy

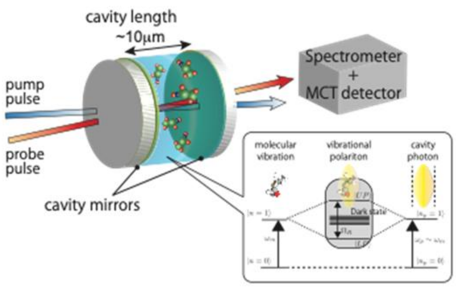

Fig. 2 formation of vibrational polaritons and ultrafast measurement scheme

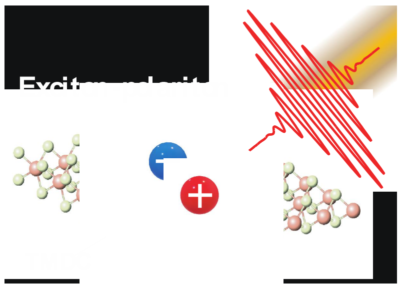

Fig. 3 ultrafast dynamics of TMDC exciton-polaritons

Staff and Contact

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Recent Research Papers and Achievements

1.Development of spacer-less flow-cell cavity for vibrational polaritons, Hayata Yamada, Garrek Stemo, Hiroyuki Katsuki, and Hisao Yanagi, J. Phys. Chem. B 126, 4689-4696 (2022).
2.Controlling ultrafast wave-packet spreading by Strong-Laser-Induced quantum interference, Hiroyuki Katsuki, Yukiyoshi Ohtsuki, Toru Ajiki, Haruka Goto, and Kenji Ohmori, Phys. Rev. Research 3, 043021 (2021).
3.Polymorph- and molecular alignment-dependent lasing behaviors of a cyano-substituted thiophene/phenylene co-oligomer,Tomomi Jinjyo, Hitoshi Mizuno, Fumio Sasaki, and Hisao Yanagi, J. Mater. Chem. C 11, 1714-1725 (2023).
4.Observation of Size-Dependent Optical Properties Based on Surface and Quantum Effects in Nanocrystals of 5,5′-Bis(4-Biphenylyl)-2,2′-Bithiophene, Tomomi Jinjyo, Hitoshi Mizuno, Kazuki Bando, Fumio Sasaki, Hisao Yanagi, Adv. Photonics Res. 3, 2100323 (2022).

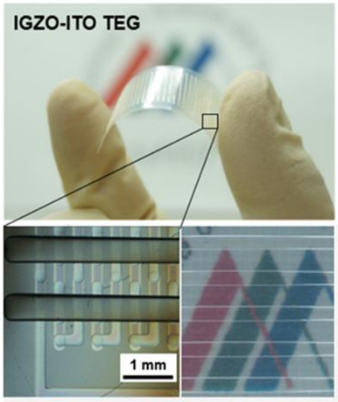
Information Device Science

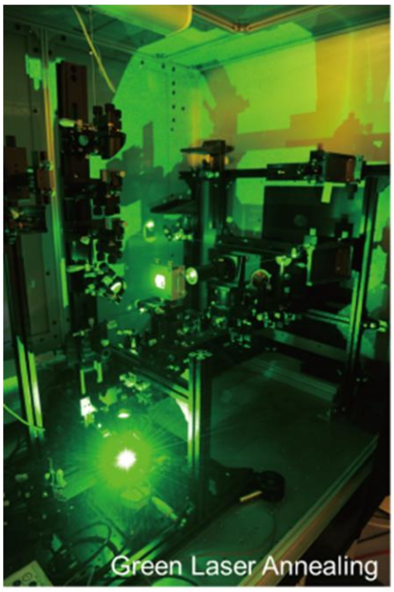
Education and Research Activities

Many daily necessities around us, such as TVs, computers, and mobile phones, are composed of silicon-based semiconductor devices. The Information Device Science Laboratory conducts research on information function devices that will support the next-generation information society. Key features of our research include the introduction of various new materials on silicon substrates, our own unique designs, and production of semiconductor devices that make the most effective use of their characteristics. Thus, we are working on producing semiconductor devices with innovative functions on the basis of skilled manufacturing.

Research Theme

1. Transparent Oxide Thin Film Transistors
2. Printed/flexible displays for wearable devices
3. Printing technology for energy harvesting devices, solar cells
4. Power devices based on GaN, diamonds.





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Recent Research Papers and Achievements

1.T. Takahashi, R. Miyanaga, M. N. Fujii, J. Tanaka, K. Takechi, H. Tanabe, J. P. Bermundo, Y. Ishikawa and Y. Uraoka, "Hot carrier effects in InGaZnO thin-film transistor", Applied Physics Express 12, 094007 (2019).
2.J. Clairvaux, M. Uenuma, D. Senaha, Y. Ishikawa, Y. Uraoka, "Growth of InGaZnO nanowires vis a Mo/Au catalyst from amorphous thin film", Appl. Phys. Lett. 111, 033104 (2017).
3.J. P. Bermundo, Y. Ishikawa, M. N. Fujii, H. Ikenoue, and Y. Uraoka, "H and Au diffusion in high mobility a-InGaZnO thin-film transistors vis low temperature KrF excimer laser annealing", Appl. Phys. Lett. 110, 133503 (2017).
4.Kahori Kise, M. Fujii, S. Urakawa, H. Yamazaki, E. Kawashima, S. Tomai, K. Yano, D. Wang, M. Furuta, Y. Ishikawa, Y. Uraoka, "Self-heating induced instability of oxide thin film transistors under dynamic stress", Appl. Phys. Lett. 108, 02501 (2016).
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6.Juan Paolo Bermundo, Yasuaki Ishikawa, Mami N. Fujii, Michel van der Zwan, Toshiaki Nonaka, Ryoichi Ishihara, Hiroshi Ikenoue, Yukiharu Uraoka, "Low Temperature Excimer Laser Annealing of a-InGaZnO Thin-Film Transistors Passivated by Organic Hybrid Passivation Layer", Appl. Phys. Lett., (2015).

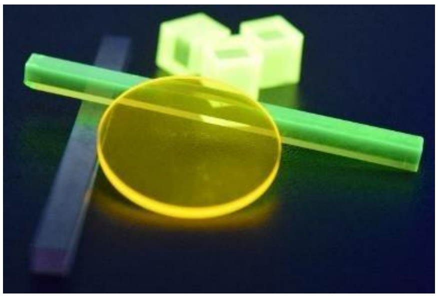
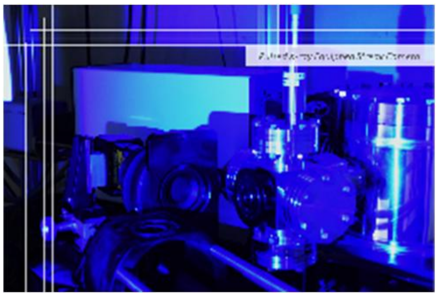
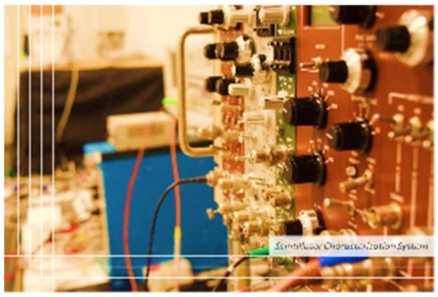
Applied Quantum Physics

Education and Research Activities

In our laboratory, students will learn skills and knowledge of radiation detection and dosimetry. We aim to enable students to independently conduct researches and publish papers in this research fields.

Research Theme

The main aim of our group is to study techniques of ionizing radiation detection and dosimetry. For this purpose, we are developing novel radiation measurement devices by using scintillators and dosimetric materials. Semiconductor detectors are also our interest as photodetectors for radiation measurement devices.

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Recent Research Papers and Achievements

1.K. Okazaki, D. Nakauchi, N. Kawano, T. Kato, N. Kawaguchi, T. Yanagida, Radiat. Phys. Chem., 202 110514 (2023).
2.H. Fukushima, D. Nakauchi, G. Okada, T. Kato, N. Kawaguchi, T. Yanagida, J. Alloys Compd., 934 167929 (2023).
3.H. Sakaguchi, H. Fukushima, T. Kato, D. Nakauchi, N. Kawaguchi, T. Yanagida, J. Lumin., 254 119533 (2023).
4.T. Hayashi , K. Ichiba, D. Nakauchi, K. Watanabe, T. Kato, N. Kawaguchi, T. Yanagida, J. Lumin., 255 119614 (2023).
5.K. Miyazaki, D. Nakauchi, T. Kato, N. Kawaguchi, T. Yanagida, Radiat. Phys. Chem., 207 110820 (2023).

Organic Electronics

Education and Research Activities

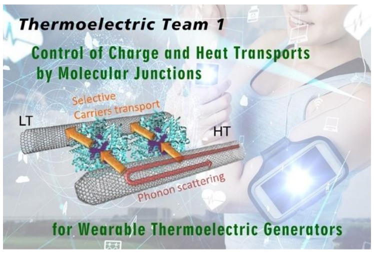
Let's imagine rollable electronic equipment, a piece of fabric generating electricity by body heat, or a paper-like solar cell. We are pursuing the realization of such novel electronic devices through studies elucidating unique phenomena in organic solids and applying the findings to the device functions using knowledge of solid-state physics, electronics, surface science, polymer physics, and molecular science. Our laboratory utilizes unique approaches made possible by our original characterization tools.
We determine individual research projects ranging from basic science to the development of real devices, depending on the student's interests and aptitudes. We foster independent thinking and a top-level mindset through collaborative research with institutes in Japan and overseas. Thus, we aim to cultivate researchers with a broad knowledge of science and a keen interest in industrial applications.

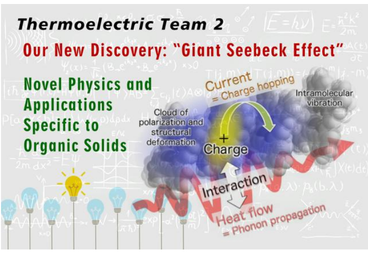
Research Theme

Three major ongoing projects are presented here, but other collaborations are underway on a spot basis.

1. Control of Charge/Heat Transports by Molecular Junctions for Wearable Thermoelectric Generators

We have demonstrated that the thermal conductivity of a carbon nanotube (CNT) composite significantly decreases by forming molecular junctions between nanotubes with a specially designed protein and other molecules. The unique character of CNT allows us to fabricate its composite yarn. With such a novel flexible thermoelectric material, we are aiming at the fabrication of "thermoelectric cloths," which can be handled like normal cloths but generate electricity from body heat.



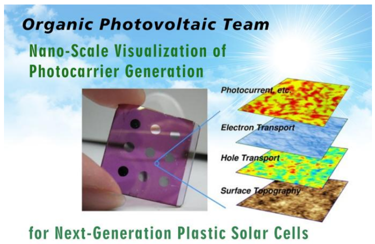


2. Basic and Applied Research on the "Giant Seebeck Effect"

We are also trying to elucidate and control the Giant Seebeck Effect in organic semiconductors discovered by us. The conventional theory of the Seebeck effect takes only the charge transport within the band theory. However, in organic semiconductors, charge and molecular vibration are strongly coupled, and thereby, the Seebeck coefficient sometimes appears to be up to 100 times larger. Not only the scientific studies, we are also developing a way to utilize this new phenomenon to produce innovative thermoelectric generators.

3. Development of Next-Generation Plastic Solar Cells

We develop next-generation "plastic" solar cells based on p- and n-type semiconducting polymers. We have been attempting to elucidate the photovoltaic properties governed by the nanoscale phase separation of polymers and the transport/recombination dynamics of photogenerated carriers with photoconductive atomic force microscopy and other techniques. Through understanding the nano-scale electronic functions, we propose new device structures that can maximize the performance.



Staff and Contact

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Web	https://mswebs.naist.jp/LABs/greendevice/www/index_e.html

Recent Research Papers and Achievements

1.M. Ito, et al., "From materials to device design of a thermoelectric fabric for wearable energy harvesters", J. Mater. Chem. A 5, 12068 (2017).
2.H. Kojima et al., "Universality of giant Seebeck effect in organic small molecules", Mater. Chem. Front. 2, 1276 (2018).
3.H. Benten et al., "Chain Aggregation Dictates Bimolecular Charge Recombination and Fill Factor of All-Polymer Blend Solar Cells" J. Mater. Chem. A 10, 21727 (2022).
4.H. Benten et al., "Nanoscale Observation of the Influence of Solvent Additives on All-Polymer Blend Solar Cells by Photoconductive Atomic Force Microscopy" ACS Appl. Polym. Mater., 4, 169 (2022).
5.M. Pandey et al., "Recent Advances in Orientation of Conjugated Polymers for Organic Field-Effect Transistors" J. Mater. Chem. C 7, 13323 (2019).
6.M. Pandey et al., "Unidirectionally aligned donor-acceptor semiconducting polymers in floating films for high-performance unipolar n-channel organic transistors", Adv. Electron. Mater., 9, 2201043 (2023).
7.M. Suda et al., "Light-driven molecular switch for reconfigurable spin filters", Nat. Commun. 10, 2455 (2019).

Photonic Device Science

Education and Research Activities

1. Laboratory outline

The Photonic Device Science Laboratory researches and develops new optical functionality-based material science and device functions for fast, flexible processing of image information that promises to play a leading role in an advanced information society and a "super aging society." Specifically, we work on applying photonic LSI technology, which integrates semiconductor circuit technology and photonic technology, toward biological and medical field applications as shown in Fig. 1. Our typical research fields include bio-medical photonic LSIs and artificial vision devices.

2. Research activity and policy

With our research subjects crossing over various research fields, we actively pursue cooperative interdisciplinary studies. For example, we are conducting joint research on artificial vision with the Department of Ophthalmology of Osaka University Graduate School of Medicine and an ophthalmologic apparatus manufacturer and also performing joint research on bio-medical photonic LSIs with the Functional Neuroscience Laboratory of NAIST.

3. Education

The majority of students in the laboratory are requested to work on research subjects involving other fields. We provide introductory seminars, study meetings, and many opportunities to interact with researchers within and outside the university so that they can pursue their research smoothly and broaden their research perspectives.

Research Theme

1. Bio-medical photonic materials and devices
2. Micro-chemical photonic devices
3. Advanced image sensors and their application systems

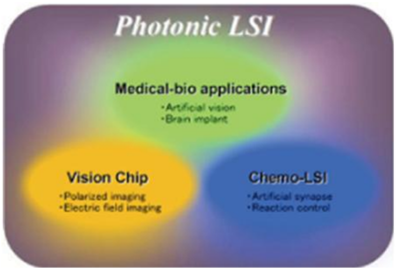

Fig. 1
Research fields of the Photonic Device Science Lab

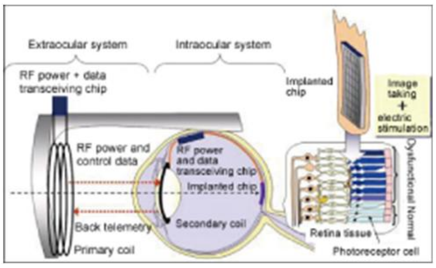

Fig. 2
Retinal prosthesis device

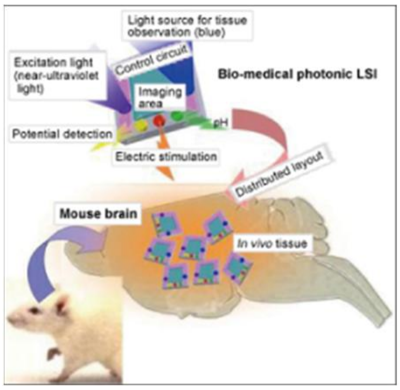

Fig. 3
Brain implantable microimager

Staff and Contact

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Recent Research Papers and Achievements

1.M. Haruta, Y. Kurauchi, M. Ohsawa, C. Inami, R. Tanaka, K. Sugie, A. Kimura, Y. Ohta, T. Noda, K. Sasagawa, T. Noda, T. Tokuda, H. Katsuki, J. Ohta, “Chronic Brain BloodFlow Imaging Device for A Behavioral Experiment Using Mice,” Biomed. Opt. Express 10, 1557, (2019).
2.J. Ohta, Y. Ohta, H. Takehara, T. Noda, K. Sasagawa, T. Tokuda, M. Haruta, T. Kobayashi, Y. M. Akay, M. Akay, “Implantable Microimaging Device for Observing Brain Activities of Rodents,” Proc. IEEE 105, 158 (2017).
3.K. Sasagawa, T. Yamaguchi, M. Haruta, Y. Sunaga, H. Takehara, H. Takehara, T. Noda, T. Tokuda, and J. Ohta, “An Implantable CMOS Image Sensor with Self-Reset Pixels for Functional Brain Imaging,” IEEE Trans. Electron Dev. 63, 215 (2016).

Thin Film Semiconductor Devices

Education and Research Activities

Our research includes the development of highly functional thin film semiconductor devices and the investigation of the physical principles linking the crystal growth, texture, and physical properties of semiconductor thin films. We employ a flexible approach to research, selecting computational, data science, and experimental approaches, including density functional theory calculations, device simulations, virtual screening of materials, thin film deposition, physical property analysis, and device fabrication. A representative outcome is the design of limiting efficiency BaSi2 solar cells using device simulation and computational material screening. By pursuing multidisciplinary research, we aim to develop researchers and engineers who are able to apply multiple approaches to issues in semiconductor devices and materials.

Research Theme

1. Solar cells
We are developing new solar cells for high efficiency, thin, rare-element-free, and low-cost devices. Materials used include $BaSi_2$, BiI_3, and SnS. Device development is accelerated by the ideal device designs enabled by device simulations and virtual screening.
2. Oxide thin film transistors
Oxide semiconductors are excellent materials that constitute efficient thin film transistors with ultralow leakage current and high mobility. We use solution combustion synthesis (SCS) to make efficient transistors by solution processes at relatively low temperatures.
3. Structure/properties of silicide semiconductor thin films
The understanding of the structure-property relationship of semiconductor thin films is essential to improve the performance of semiconductor devices. We apply our original thin film deposition technique to Zintl-phase semiconductors to deepen the fundamental understanding of semiconductor thin films.
4. Group-IV 2D nanosheets
Group-IV 2D nanosheets are a class of layered semiconductors having attractive properties such as high theoretical carrier mobility and large band gaps. To pioneer the applications to high performance semiconductor devices, we are studying thin film synthesis techniques and physical properties.

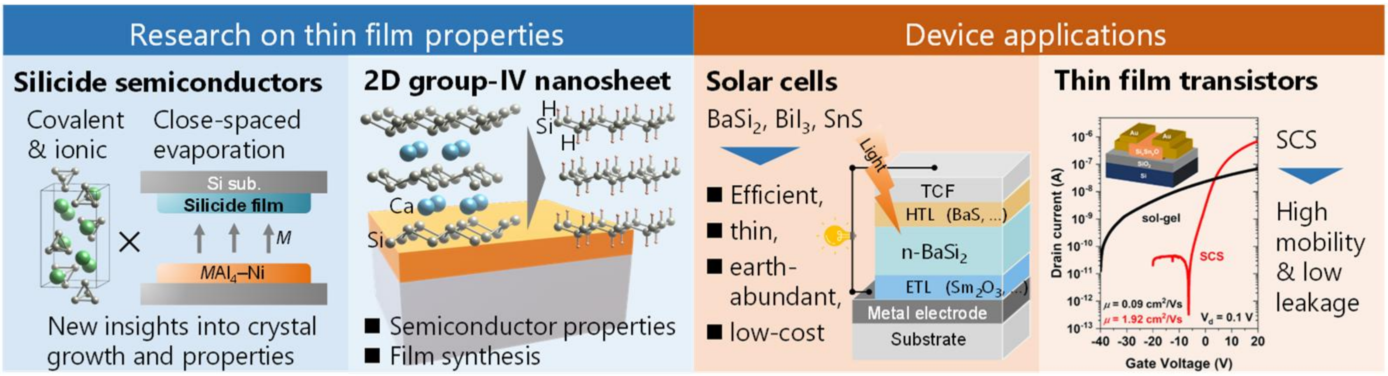

Fig. Outline of research activities, including investigations into thin film properties and the development of semiconductor devices.

Staff and Contact

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Recent Research Papers and Achievements

1. K. O. Hara, et al., J. Alloys Compd. 966, 171588 (2023).
2. K. O. Hara, Sol. Energy 245, 136 (2022).

Photonic and Reactive Molecular Science

Education and Research Activities

Our laboratory focuses on *Photonic and Reactive Molecular Science*—an emerging interdisciplinary field that investigates molecules and coordination compounds with advanced photo-functional and reactive properties. We develop novel photo-reactive and light-emissive molecules, along with innovative synthetic methodologies and catalytic systems. Students in our lab gain hands-on experience in synthetic organic chemistry, while also engaging in the development of new molecular systems and catalytic processes. A background in organic chemistry, physical chemistry, and/or spectroscopic techniques is recommended for prospective members. We warmly welcome motivated students from both domestic and international universities with backgrounds in chemistry or related fields. Our current research interests include the following:

Research Theme

1. Photoresponsive Molecules and Photoreactions

Photochromic terarylenes are among the most extensively studied compounds in our group. In addition to their use as color-changing materials, we are actively developing novel photoswitchable and light-responsive systems. For example, we explore the photo-controlled behavior of supramolecular aggregates and their fluorescence properties as key research themes. Our work also involves the development of new photo-induced catalysts based on photochromic terarylenes, as well as a newly designed naphthoquinone-based photo-labile molecular platform. These photoreactive molecules hold potential for applications in next-generation radiation-sensing materials, stimuli-responsive medical agents, and photoresist and photocuring technologies.

2. Intelligent luminescent Molecules

Photoluminescent molecules are widely used and continuously developed for next-generation display technologies, light-emitting devices, sensors, functional inks, and security markings. In our group, we design novel luminescent materials with advanced "intelligent" functionalities to contribute to the future of materials chemistry. Our current focus includes chiral luminescent molecules and coordination compounds capable of emitting circularly polarized light—promising candidates for use in security inks and specialized optical applications. Additionally, we have recently developed molecular systems exhibiting delayed luminescence and inverted triplet energy levels, offering great potential as highly efficient light sources.

3. Advanced catalysts and reaction systems for efficient organic synthesis

The development of novel organic synthetic reactions is also a key research focus in our laboratory. In particular, we are exploring new reactions mediated by transition metal complexes, acids, and bases with the aim of activating and cleaving inert bonds in synthetically and industrially relevant molecules. Our ultimate goal is to synthesize (photo) functional compounds and investigate their properties using these newly established methodologies.

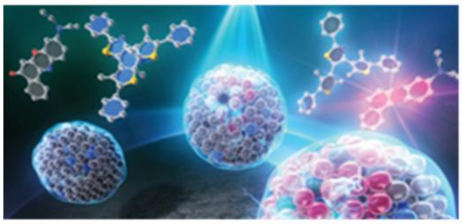

Fig.1
Novel molecules with high light, ionixc and radiation sensitivity.

Fig.2
New organic transformations enabling carbon neutrality

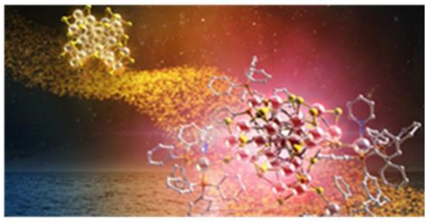

Fig.3
NIR-emissive Ag29 Nanoclusters: surface coordination chemistry and chirality control

Staff and Contact

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Recent Research Papers and Achievements

1. M. Yamada, T. Sawazaki, M. Fujita, F. Asanoma, Y. Nishikawa, T. Kawai, "Tetrathienyl corannulene compounds with highly sensitive photochromism", *Chem. Eur., J*, 28, e202201286 (2022).
2. Y. Tsuji, N. Kanno, C. Goto, S. Katao, Y. Okajima, P. Reine, P. Imbrasas, S. Reineke, K. Shizu, T. Nakashima, H. Kaji, T. Kawai, M. Louis," A binaphthalimide motif as a chiral scaffold for thermally activated delayed fluorescence with circularly polarized luminescence activity", *J. Mater. Chem. C*, 11, 5968 (2023).
3. E. Hayashi, N. Akiyama, K. Kakiuchi, T. Kawai, T. Morimoto, "Cationic Rhodium (I) - Catalyzed Asymmetric Cyclohydroformylation of 1, 6 - Enynes with Formaldehyde", *Chem.-An Asian J.*, 18, e202201241 (2023).
4. W. Ishii, Y. Okayasu, Y. Kobayashi, R. Tanaka, S. Katao, Y. Nishikawa, T. Kawai, T. Nakashima, "Excited State Engineering in Ag_{29} Nanocluster through Peripheral Modification with Silver(I) Complexes for Bright Near-Infrared Photoluminescence", *J. Am. Chem. Soc.*, 145, 11236 (2023)
5. Y. Higashi, K. Shima, M. Suzuki, M. Fujishiro, T. Kawai, T. Morimoto, "Synthetic Utilization of 2*H*-Heptafluoropropane: Ionic 1,4-Addition to Electron-Deficient Carbon–Carbon Unsaturated Bonds" *J. Org. Chem.*, 89, 3962 (2024).
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7. R. Sethy, A. Brosseau, T. Nakashima, T. Kawai, R. Métivier, "Fluorescence Microscopy Imaging of Light-Harvesting in Self-Assembled Nanofibers of Naphthalenediimides toward Perylenediimide Guests" *ACS Appl. Mater. Interfaces*, 17, 10976 (2025)

Biomimetic and Technomimetic Molecular Science

Education and Research Activities

There are no physical limitations to the miniaturization of a machine down to the scale of a single molecule or conversely, to monumentalize a molecule until it becomes a machine. A molecular machine is a molecule designed to perform a function providing energy, data or/and orders to the molecule. Inspiration from mother nature and from modern technologies has given rise to the concept of biomimetic and technomimetic molecular machines respectively. Also, synthetic mimics of natural molecular machines in biological systems will contribute to clarifying the minimal design of biologically-active agents.

The Biomimetic and Technomimetic Molecular Science Laboratory studies molecules which can act as machines at the nanoscale. Thanks to an input signal as an energy source (light, electron, or chemical) these molecular machines can produce a controllable motion and then to a useful output.

Research Theme

1. Technomimetic molecular machines

Technomimetic molecular machines are molecules designed to imitate macroscopic objects at the molecular level, and also to transpose the motions that these objects are able to undergo. Our originality is in the design of molecular machines and devices operating at the atomic scale for molecular mechanical applications: gears,[1] vehicles,[2] etc. We are designing, synthesizing, organizing and synchronizing such molecular nanodevices to develop energy, communication and information transfer at the nanoscale under the action of light, heat or electrons.

2. Biomimetic molecular machines

Biomimetic molecular machines are molecules inspired by nature. For instance, ATP-synthase is a fantastic motor present in all the cells to stock energy by converting ADP in ATP during a clockwise rotation of the rotor subunit while it can also release energy on-demand by hydrolyzing ATP in ADP through a counterclockwise rotation. This biomolecular motor inspired us to design and synthesized a molecular analog 20 times smaller in size but with a similar behavior.[3] We also design Hybrid molecular machines[4] to build new generation molecular machines and materials. Insertion of photoactive or electroactive molecular devices in membranes or in cells may induce some interesting biological activities.

3. Mimetics of proteins / peptides by synthetic polymer

Proteins and peptides are essential macromolecules necessary for various biological functions in living systems. Our challenge is to establish a design principle of synthetic polymers that express biological activities by mimicking natural proteins or peptides. We have been developing membrane-active polymers that can express biological activities such as antimicrobial[5], anticancer, and antiamyloid. Also, a series of amphiphilic polymers or lipids have been designed for the fabrication of an artificial cell membrane[6].

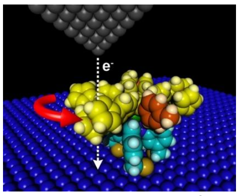

Fig. 1

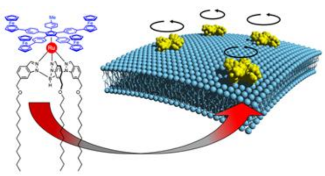

Fig. 2

Fig. 3

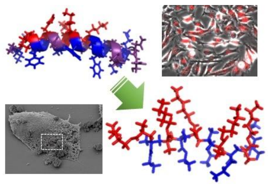

Fig. 4

Fig. 1 A Molecular motor rotating clockwise or counterclockwise by request.
Fig. 2 Modulation of cell membrane structure by biomimetic molecular machines.
Fig. 3 Molecular nanovehicle at the Nanocar Race 2 (March 2022)
Fig. 4 Mimetics of protein / peptide by synthetic polymer

Staff and Contact

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Recent Research Papers and Achievements

1.*Extended tripodal hydrotris(indazol-1-yl)borate ligands as ruthenium-supported cogwheels for on-surface gearing motions.* K. Omoto, M. Shi, K. Yasuhara, C. Kammerer, G. Rapenne, Chem. Eur. J. 2023, 29, e202203483.

2. *A dipolar nanocar based on a porphyrin backbone* T. Nishino, C. Martin, H. Takeuchi, F. Lim, K. Yasuhara, Y. Gisbert, C. Kammerer, G. Rapenne, Chem. Eur. J. 2020, 26, 12010.

3. *Controlled clockwise and anticlockwise rotational switching of a molecular motor* G. Rapenne, S.-W. Hla et al, Nature Nanotech. 2013, 8, 46.

4. *A molecular motor functionalized with a photoresponsive brake* R Asato, C.J. Martin, Y. Gisbert, F. Asanoma, T. Nakashima, C. Kammerer, T. Kawai, G. Rapenne, Inorg. Chem. 2021, 60, 3492.

5. *Mechanistic Study of Membrane Disruption by Antimicrobial Methacrylate Random Copolymers by the Single Giant Vesicle Method* M. Tsukamoto, E. Zappala, G. A. Caputo, J. Kikuchi, K. Najarian, K. Kuroda, K. Yasuhara, Langmuir 2021, 37, 9982-9995.

6. *Synthetic mimics of membrane-active proteins and peptides* K. Yasuhara, in Plasma membrane Shaping, Elsevier, 2022, pp.159-173.

Functional Organic Chemistry

Education and Research Activities

We focus on the development of functional organic materials including organic semiconductors, highly fluorescent dyes, near-infrared (NIR) dyes, and carbon nanomaterials. In particular, we are fascinated by beautiful and huge organic structures with high symmetry. We are also interested in the control of self-assembled structures to achieve their synergistic performances. Students at our laboratory are encouraged to work independently and freely on their own original research themes.

Research Theme

1. Creation of unique carbon frameworks with beautiful shapes and novel functionality

We are developing new synthetic methods for polycyclic aromatic hydrocarbons such as nanocarbons and oligorylenes, which have a unique shape and are chemically stable with an extended π-conjugated system (Fig. 1, 2).

2. Molecular design of novel nanocarbon materials with absorption and emission in the near-infrared region

We are interested in designing molecules with long wavelength absorption and luminescence (Fig. 3). As an unusual example, we have successfully created a luminescent molecule in the near-infrared region by using fullerene C70, traditionally used as electron-accepting materials. We observed circularly polarized luminescence (CPL) of a chiral C70 derivative for the first time (Fig. 4). We are also synthesizing highly efficient light-emitting materials by taking advantage of the characteristics of the triplet excited state species.

3. Construction of carbon nanocages with robust structure

We aim to synthesize quantum dot clusters with atomic precision by performing chemical reactions in nanocages constructed by bottom-up organic synthesis using planar panel units.

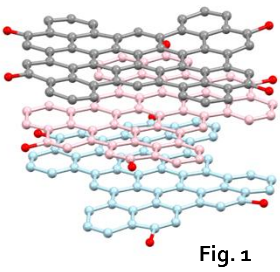

Fig. 1

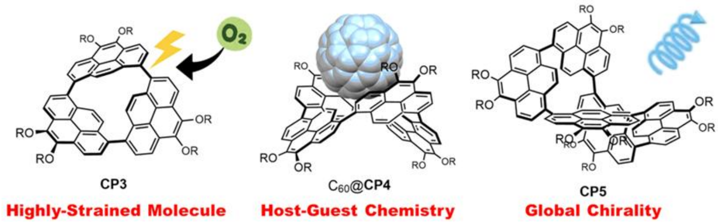

Fig. 2

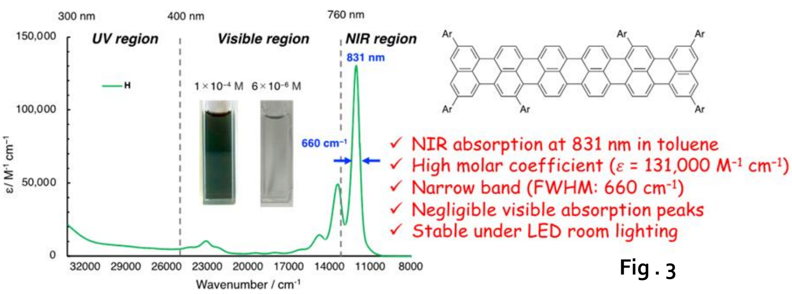

Fig . 3

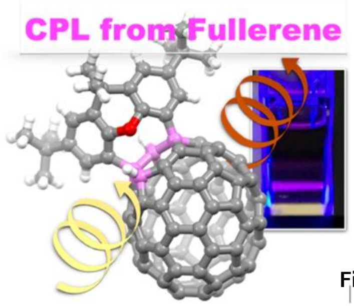

Fig. 4

Staff and Contact

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Recent Research Papers and Achievements

1.N. Aratani, et al., Tetrabenzoperipentacene: Stable Five-Electron Donating Ability and a Discrete Triple-Layered β-Graphite Form in the Solid State, Angew. Chem. Int. Ed. 2015, 54, 8175.
2.N. Aratani, et al., A remarkably strained cyclopyrenylene trimer that undergoes metal-free direct oxygen insertion into the biaryl C-C δ-bond, Chem. Sci. 2019, 10, 6785.
3.N. Aratani, et al., Torsional chirality generation based on cyclic oligomers constructed from an odd number of pyrenes, Chem. Commun. 2019, 55, 9618.
4.N. Aratani, et al., A Series of Soluble Planar Oligorylenes up to Hexarylene, Chin. J. Chem. 2023, 41, 1023.
5.N. Aratani et al., Deep-red circularly polarised luminescent C_{70} derivatives, Sci. Rep., 2021, 11, 12072.

Functional Inorganic Materials Design

Education and Research Activities

Ceramic materials play a vital role across a wide range of fields, including manufacturing, infrastructure, electronics, energy, medical, and environmental technology. In order to realize a sustainable society, it is essential to develop technologies that minimize the environmental impact of material synthesis, enable efficient production using limited resources and energy, and improve their performances through innovation. Our research group focuses on environmentally friendly ceramics synthesis via liquid-phase processes. We aim to develop novel synthesis methods and to finely tune the functional properties of ceramics for advanced applications such as environmental purification, biomaterials, and chemical sensors. Through these research activities, we aim to nurture researchers and engineers who can take on the challenges of realizing our vision for the future.

Research Theme

- Novel liquid-phase synthesis processes for controlling crystal phase, morphology, and orientation (Fig. 1)
- Sorbents or ion-exchangers for environmental remediation and resource recovery (Fig. 2)
- Upcycled functional materials from used, waste or unused resources
- Functional properties of bioceramics by controlling crystallographic properties

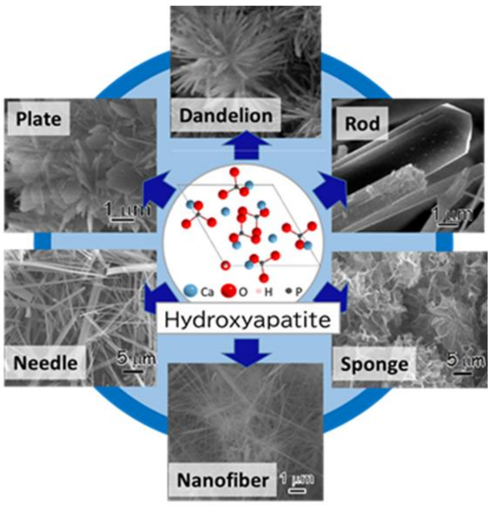

Fig. 1 Crystal morphology of hydroxyapatite synthesized by hydrothermal method

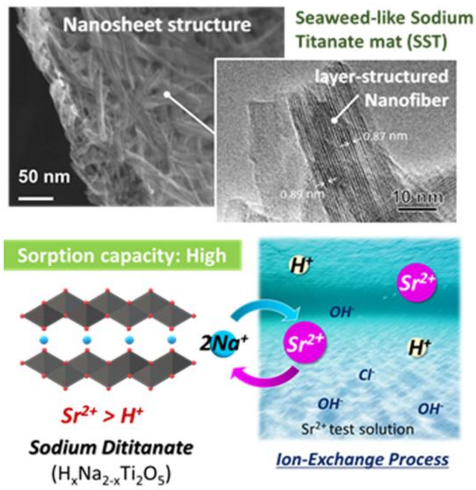

Fig. 2 Inorganic ion-exchanger with hierarchical nanostructure for water treatment

Staff and Contact

	Educational Staff	Prof. Tomoyo Goto
	Web	

Recent Research Papers and Achievements

T. Goto*, S. Yin, Y. Asakura, S. H. Cho, T. Sekino, Simultaneous synthesis of hydroxyapatite fibres and β-tricalcium phosphate particles via a water controlled-release solvothermal process, *CrystEngComm* **25** (2023) 2021-2026.
T. Goto*, Y. Kondo, S. H. Cho, S. Seino, T. Sekino, Comparative study of divalent cation sorption on titania nanotubes using Co^{2+}, Ni^{2+}, Zn^{2+}, and Sr^{2+}, *Chem. Eng. J. Adv*. **12** (2022) 100388.
Y. Kondo, T. Goto*, T. Sekino*, Sr^{2+} sorption property of seaweed-like sodium titanate mats: effects of crystallographic properties, *RSC Adv*. **11** (2021) 18676-18684.
T. Goto*, S. H. Cho, C. Ohtsuki, T. Sekino, Selective adsorption of dyes on TiO_2-modified hydroxyapatite photocatalysts morphologically controlled by solvothermal synthesis, *J. Environ. Chem. Eng*. **9** (2021) 105738.

Functional Supramolecular Chemistry

Education and Research Activities

We are performing new interdisciplinary researches in chemistry and biology. Based on the chemical knowledge of the functions and structures of biomolecules at molecular level, our laboratory focuses on the elucidation of protein mechanisms and design/application of bio-supramolecules using various analytical methods, protein engineering techniques, and organic syntheses.

Research Theme

1. New protein drug development

We make new protein drugs from human antibody light chains. We also design and make artificial proteins with multi-active sites exhibiting antibacterial activity (Fig. 1). These protein drugs are attracting attention in the biotechnology and pharmaceutical science fields.

2. Bio-supramolecule creation

It would be extremely useful for life if we could create new proteins as we like. For this purpose, we construct new protein supramolecules by introducing a new design method in which building block proteins are used as structural units (Fig. 2).

3. Relationship between disease and protein denaturation mechanism

Accumulation of proteins with unusual structures in tissues causes various diseases such as abnormal hemoglobin disease, Alzheimer's disease, and Parkinson's disease (conformational diseases). We investigate denaturalization of these proteins at the molecular level and develop strategies to inhibit the denaturalization. We also study the aggregation process of antibodies.

4. Functionalization of proteins by synthetic chemistry

We develop novel biocatalysts and artificial proteins using synthetic chemistry and biochemical approaches. The functionalized proteins will be applied for organic syntheses and regulation of naturally occurring bioreactions (Fig. 3). In this view, we synthesize novel synthetic compounds that are hybridized with biomolecules.

5. Functional analysis of interaction fashions between biomolecules for medicinal chemistry

To understand and regulate bioreactions, we develop methods for bioreaction regulation based on interactions between biomolecules from the perspective of medicinal chemistry and chemical biology.

6. Computer-based protein design

We design functional proteins using deep learning and purify them by wet experiments.

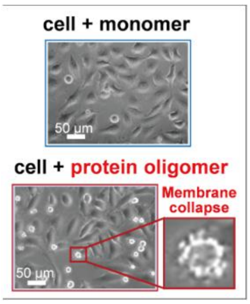

Fig. 1
Creation of antibacterial protein supramolecules

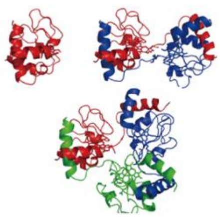

Fig. 2
Elucidated structures of cytochrome c supramolecules

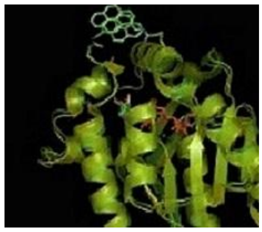

Fig. 3
X-ray crystallographic structure of an artificial fluorescent protein constructed by a combination of genetic and synthetic methods

Staff and Contact

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Recent Research Papers and Achievements

1.M. Zhang et al., *J. Phys. Chem. B*, 127, 2442 (2023).
2.S. Hirota et al., *Chem. Commun.*, 58, 12839 (2022).
3.S. T. Stripp et al., *Chem. Rev.*, 122, 11900 (2022).
4.H. Tai et al. , *Acc. Chem. Res.*, 54, 232 (2021).
5.S. Hirota, et al. *Chem. Commun.,* 57, 12074 (2021) (Future Article).
6.S. Hirota, S. Nagao, *Bull. Chem. Soc. Jpn.*, *94*, 170 (2021) (Award Account, Inside Cover)
7.C. Xie et al., *RSC Advances, 11*, 37604 (2021).
8.M. Yamanaka et al., *PLoS One*, *16*, e0259052 (2021).
9.S. Nagao et al., *J. Inorg. Biochem.*, *217*, 111374 (2021).
10.S. Nagao et al., *Chem. Asian J.*, 15, 1743 (2020) (Very Important Paper).
11.H. Tai, S. Hirota, *ChemBioChem*, 21, 1573 (2020) (Very Important Paper).
12.T. Miyake, T. Matsuo et al., *Bioconjugate Chem.*, 31, 794 (2020).
13.R. Cahyono et al., *Metallomics*, 12, 337 (2020) (Front Cover)

Complex Molecular Systems

Education and Research Activities

The concerted actions of various molecules result in high-order functions that cannot be realized by individual molecules, as seen in various biological systems. The Complex Molecular Systems Laboratory, established on April 1, 2015, currently focuses on the complex molecular systems involving multicomponent biological molecules such as proteins. Weakly and/or strongly coupled proteins undergo regulatory dissociation and association in response to external stimuli, thereby exhibiting advanced biological functions. To determine the physicochemical properties of these molecular systems and to create new functional molecular systems, our laboratory employs various biophysical techniques, such as structural analysis using multiple probes (X-ray, neutron, and electron), spectroscopic measurements, protein engineering, and theoretical analysis. Multidisciplinary knowledge is essential to clearly understand the characteristics of these complex molecular systems. We welcome students with various educational backgrounds such as physics, chemistry, material science, and biology. By enabling students to work on their own research theme independently, we encourage them to develop their own interests and to learn essential research skills, such as identifying problems to be solved, designing experiments that will yield solutions, and comprehensively interpreting experimental results.

Research Theme

1. Development of analytical methods to investigate complex molecular systems (Fig. 1)
2. Investigation of the dynamical ordering of multi-component proteins (Fig. 2)
3. Creation of high-order self-assembled complex molecular systems (Fig. 2)
4. Detailed analysis of intramolecular actions in individual proteins responsible for the dynamical ordering of complex molecular systems in higher-class structural hierarchy (Fig. 3)
5. Development of rational molecular designs for novel synthetic proteins

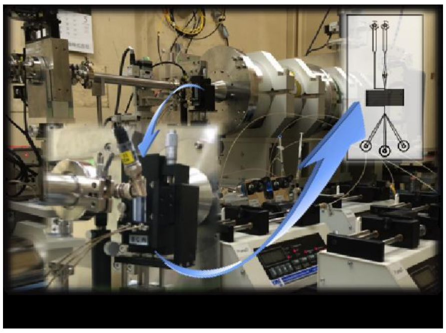

Fig. 1
Micro-fluidics based analyzer equipped for structure/interaction analysis of complex molecular systems

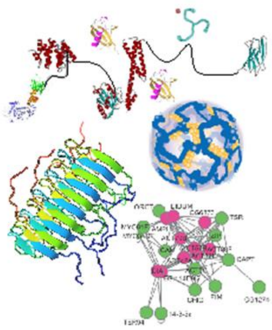

Fig.2
Biological complex molecular systems

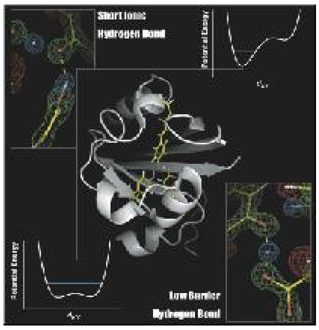

Fig.3
Protonics in protein molecules

Staff and Contact

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Recent Research Papers and Achievements

1.K. Yonezawa, N. Shimizu, K. Kurihara, Y. Yamazaki, H. Kamikubo, M. Kataoka. "Neutron crystallography of photoactive yellow protein reveals unusual protonation state of Arg52 in the crystal." *Sci Rep* 7(1):9361. (2017).
2.H. Kuramochi, S. Takeuchi, K. Yonezawa, H. Kamikubo, M. Kataoka, T. Tahara, "Probing the early stages of photoreception in photoactive yellow protein with ultrafast time-domain Raman spectroscopy", *Nature Chemistry*, 10.1038/nchem.2717 (2017).
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4.F. Schotte, H. S. Cho, V. R. I. Kaila, H. Kamikubo, N. Dashdorj, E. R. Henry, T. J. Graber, R. Henning, M. Wulff, G. Hummer, M. Kataoka, P. A. Anfinrud, "Watching a signaling protein function in real time via 100-ps time-resolved Laue crystallography", *Proc. Natl. Acad. Sci. USA* 109 19256-19261 (2012).
5.S. Yamaguchi, H. Kamikubo, K. Kurihara, R. Kuroki, N. Niimura, N. Shimizu Y. Yamazaki, M. Kataoka, "Low-barrier hydrogen bond in photoactive yellow protein", *Proc. Natl. Acad. Sci. USA* 106 440-444 (2009).

Nanomaterials and Polymer Chemistry

Education and Research Activities

Based on the concept of "molecular technology", this laboratory was established in 2015 to conduct functional polymer materials research in the field of polymer chemistry. The laboratory transitioned as one of core laboratory at Materials Science Division at NAIST in 2019. Students who are interested in polymer synthesis and nanomaterials are welcome. The development of functional polymer materials requires various knowledge including organic synthesis, analytical methods, and materials design, all of which are covered in the laboratory. Moreover, our functional materials will contribute to medical devices, energy related materials, and environmentally friendly polymer materials. We offer a thorough education through discussions, presentations, and participation in academic conferences and meetings so that students become qualified researchers.

Research Theme

In this laboratory, high-performance polymers and functional polymers are prepared by various approaches such as molecular design, polymer structure control, and effective polymer-polymer interaction.

1. Control of Polymer Structure

Precise polymerization, flow system, and material processing are utilized in order to create the novel polymer structure and material. For example, star- and cage- shaped polymers, as well as narrow PDI, by living radical polymerization, well-defined and cyclic polymers by development of novel polymerization methods, and non-woven fabric with low molecular weight compounds by electrospinning process method.

2. Degradable Polymer

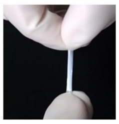
Molecular design of the novel monomers contribute to medical and environment. For example, medical materials, long-term drug release, and environmentally friendly polymers are created by poly(trimethylene carbonate derivative)s with ester free structure, polylactides with chain end modification, and chemically modified poly(butylene succinate) with double bond in the main chain.

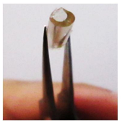
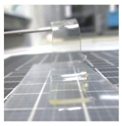
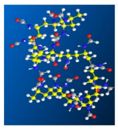
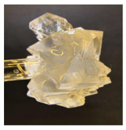
3. High Performance Polymer

For the alternative of general polymers, new amphiphilic polymers and natural polymers are utilized to control mechanical strength or thermal properties. For example, molecular weight and particle control by N-vinylamide, flexible materials, resin altenative, antifouling surfaces, and surface control by chitin, cellulose, agarose are designed and prepared.

4. Novel Functional Polymer

Molecular technology concept contribute to the creation of next- generation functional materials. For example, water-harvesting, surface-covered, highly-stretching, and water-retaining materials by functional hydrogels, thermal storage by nanofilm coating, and novel functional materials by stereocomplex are created.



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Recent Research Papers and Achievements

1.Nalinthip Chanthaset*, Akari Maehara, Hiroharu Ajiro*, “Particles and film preparation of ester-free type poly(trimethylene carbonate) derivatives bearing aromatic groups initiated with hydrophilic initiators”, Colloids Surf. A. 2023, 667(20), 131413(8).
2.Lee Yae Tan, Nalinthip Chanthaset*, Arif Fadlan, Hiroharu Ajiro,* “Synthesis of Ester-free Poly(trimethylene carbonate) Bearing Cinnamyl Moiety for Antibacterial Biomaterials Applications”, React. Funct. Polym., 2023, 186, 105563(8).
3.Kamolchanok Sarisuta, Mizuho Iwami, Blanca Martin-Vaca, Nalinthip Chanthaset*, Hiroharu Ajiro*, “The pH Effect on Particle Aggregation of Vanillin End-capped Polylactides Bearing Hydrophilic Group Connected by Cyclic Acetal Moiety”, Langmuir, 2023, 39, 3994-4004.
4.Tsuyoshi Ando*, Kazuki Yamaguchi, Hiroharu Ajiro,* “Thermoresponsive star-shaped polymer with heteroarm type with methacrylates prepared by living radical polymerization method”, Polym. Chem. 2023, 14, 1027-1035.
5.Miguel Palenzuela, KamolchanokSarisuta, Marta Navarro, Narumi Kumamoto, Nalinthip Chanthaset, Julien Monot, Hiroharu Ajiro, Blanca MARTIN-VACA,* Didier Bourissou* “5-Methylene-1,3-Dioxane-2-One: A First Choice Comonomer for Trimethylene Carbonate”, Macromolecules, 2023, 56(2), 678-689.
6.Ryo Kawatani, Taiga Hamawaki, Tomonori Waku, Naoki Tanaka, Hiroharu Ajiro*, “Evaluation of Biocompatible Films using Copolymers of N-Vinylbenzamide with Cationic Moieties by Hydrolysis of N-Vinylformamide”, Macromol. Chem. Phys. 2023, 2200386.
7.Izabela Kurowska, Alexis Dupre-Demorsy, Stéphane Balayssac, Marie Hennetier, Audrey Ric, Valérie Bourdon, Tsuyoshi Ando, Hiroharu Ajiro, Olivier Coutelier, Mathias Destarac*, “Tailor-made poly(vinylamine) via purple LED-activated RAFT polymerization of N-vinylformamide”, Macromol. Rapid Commun. 2023, 2200729 (6), OPEN ACCESS.
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9.Alexis Dupre-Demorsy, Izabela Kurowska, Stéphane Balayssac, Marie Hennetier, Audrey Ric, Valérie Bourdon, Tsuyoshi Ando, Hiroharu Ajiro, Olivier Couteliera, Mathias Destarac*, “RAFT polymerisation of N-vinylformamide and corresponding double hydrophilic block copolymers”, Polym. Chem. 2022,13, 6229-6237.
10.Lee Yae Tan, Nalinthip Chanthaset*, Hiroharu Ajiro*, “Surface Coating and Characteristics of Ester-free Poly(trimethylene carbonate) Bearing an Aromatic Urea Moiety for Biomaterials Use”, Mater. Adv. 2022, 3, 5778-5785.
11.Daisuke Aoki, Francisco Lossada, Daniel Hoenders, Hiroharu Ajiro*, Andreas Walther*, “Efficient softening and toughening strategies of cellulose nanofibril nanocomposites using comb polyurethane”, Biomacromolecules 2022, 23, 1693-1702.
12.Rikyu Miyake, Akari Maehara, Nalinthip Chanthaset, Hiroharu Ajiro*, “Thermal property control by copolymerization of trimethylene carbonate and its derivative bearing triphenylmethyl group”, ChemistrySelect 2022, 7, e202104326.
13.Alexis Dupre-Demorsy, Olivier Coutelier, Mathias Destarac*, Clémence Nadal, Valérie Bourdon, Tsuyoshi Ando, Hiroharu Ajiro, “RAFT Polymerization of N-Methyl-N-Vinylacetamide and Related Double Hydrophilic Block copolymers”, Macromolecules 2022, 55, 1127-1138.
14.Hiroaki Yoshida*, Hiroya Furumai, Hiroharu Ajiro*, “Preparation and Characterization of Thermoresponsive Poly(N-vinylisobutyramide) Microgels” Langmuir, 2022, 38, 5269-5274.
15.Shin Asano, Jaeyeong Choi, Tran Thi Tran, Nalinthip Chanthaset, Hiroharu Ajiro*, “The influence of chain-end functionalization and stereocomplexation on the degradation stability under alkaline condition” Polym. Adv. Technol. 2022, 33(3), 991-999.

Materials Informatics

Education and Research Activities

Recent progress in the research filed of the machine learning and artificial intelligence bring us a new filed of materials sciences, called "materials informatics". This is attracting attention as the fourth science following experimental sciences, theoretical sciences, and computing sciences. We will promote studies on materials informatics, aiming to build new principles in material sciences and accelerate materials development.

The basic concept of materials informatics is a closed loop consisting of data collection, construction of learning models, search in design space, and experiments. Here, we will build a learning theory that extracts the essential principles common to multiple materials and multiple physical properties, and enable the essential understanding of materials and prediction of physical properties of new materials. Furthermore, we will develop methodologies to design new materials with desired properties by advancing Bayesian optimization and sequential learning, which are one of the design of experiments, and generative models. In addition to developing these new theories and algorithms, our laboratory will promote joint studies with experimental research groups and demonstrate the acceleration of material development.

Research Theme

1. Learning methodology for multiple materials and multiple physical properties: The recent progresses of the materials informatics in this decade enabled to learn and predict individual properties. We will advance the learning models to multiple materials and multiple physical properties, which resolve limited data problem in the material sciences and promote materials development.

2. Theoretical and computational designing of new materials: Material design with a desired physical property is a milestone in the material sciences. We will develop methodologies for expressing and generating material information leading to the material design based on crystal structures. Here, in addition to the materials informatics, theoretical and computational chemistry techniques are also incorporated to develop the methodologies.

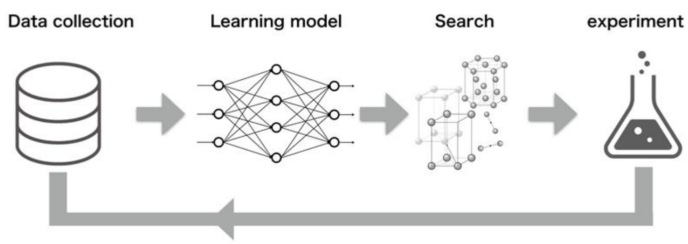

Fig. 1: Basic concept of Materials Informatics that is a closed loop consisting of data collection, construction of learning models, search in design space, and experiments

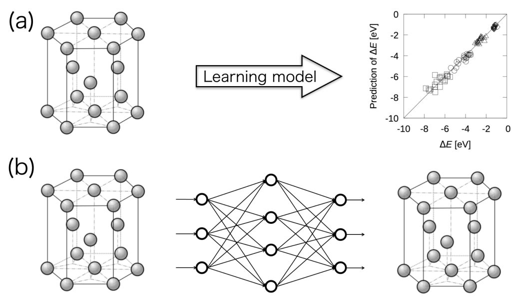

Fig. 2: Schematic view of (a) learning and predicting physical properties and (b) generative models (e.g., autoencoder) of crystal structure

Staff and Contact

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Data Driven Chemistry

Education and Research Activities

Chemoinformatics is a research area where chemical problems are tackled using tools coming from informatics. Our mission is to develop chemoinformatics tools that are truly useful and practical for applications in the field of chemistry. For example, molecular representations have been extensively investigated for virtual screening of a large compound data set for identifying bioactive compounds. Likewise, the investigation of appropriate chemical reaction representations for predicting reaction parameters (yield, selectivity) is a current research activity. For developing tools or methods, one must understand both domain knowledge (chemistry or biology) and analysis techniques (statistics, machine learning). Either having experienced one of the two studies is preferable for conducting meaningful research. So far, most of the students in our group have chemistry or biology- backgrounds. They have learned information techniques through a training program provided by our group. Starting from the basics of data analysis (machine learning), you will learn how to handle chemistry-related data and analyze them to obtain useful information. For students who have an information-science background, they can learn knowledge of chemistry and biology focusing on drug discovery to conduct meaningful study.

Research Theme

1.Methodology development for affinity prediction

Virtual screening is a process that selects potential candidate compounds for a specific target from a compound pool. In ligand-based approaches, the principle that similar compounds show similar biological activity holds. This principle, however, is not necessarily true when focusing on ligand-protein binding mechanisms. Methodology development for extracting key information for this phenomenon in ligand-based approaches furthers improvement of virtual screening.

2.Constructing high predictive soft sensor models using limited data sources

Predicting chemical reaction parameters (yield or selectivity) in advance can contribute not only to reducing experimental costs but also to understanding the reaction mechanism. Once we understand the reaction, optimal experimental conditions (including catalysts) can be proposed. Since data for organic chemical reactions have been accumulated, these data should be utilized effectively.

3. Modeling approaches in Low data regime

Laboratory-scale chemistry data sets are small: less than 50 samples (sometimes around 10), which were experimented at a homogenous experimental condition. Mechanism-oriented molecular representation in combination with traditional machine learning modeling would be a reasonable approach for this type of problem, however, recently develop DNN techniques: meta-learning, pre-training would also be options.

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Recent Research Papers and Achievements

1.S. Shibayama, H. Kaneko, K. Funatsu, Comput. Chem. Eng. 113, 86-97, 2018
2.T. Miyao, K. Funatsu, J. Bajorath, F1000Research, 2017, 6 :1285
3.T. Miyao, H. Kaneko, K. Funatsu, J. Chem. Inf. Model., 2016, 56, 286-299

Metrology Informatics

Education and Research Activities

While considering students' backgrounds and motivations, we set themes related to metrology technology and materials analysis, which are indispensable for the research and development of advanced functional materials and devices. We aim to cultivate problem-solving skills by pursuing the essentials using information science and computer simulations. In addition, through joint research with other organizations and participation in academic conferences at domestic and abroad, we cultivate the ability to think from a broad perspective.   In our laboratory, we develop material analysis and measurement techniques necessary for realizing next-generation advanced materials and devices while entirely using information science. We also aim to solve various problems in the research and development of advanced materials and devices using the developed methods. Research themes will be actively pursued as joint research inside and outside the university.

Research Theme

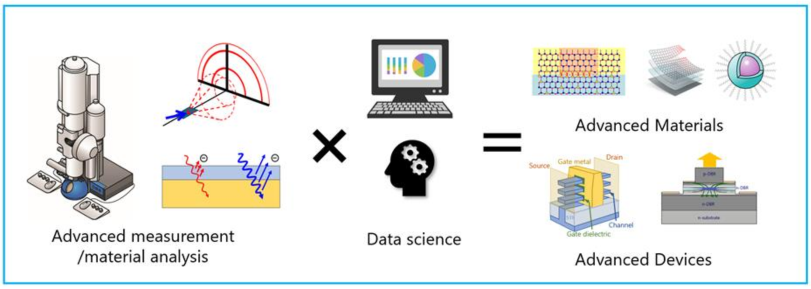
1. Multimodal Metrology

Advanced functional devices are indispensable for social infrastructure systems that must be more sophisticated and energy-efficient. In line with this trend, device structures and fabrication processes are becoming more complex, and introducing new materials is essential to add new functions. Such R&D requires the development and introduction of further analysis and measurement techniques. Furthermore, it is necessary to combine multiple analysis and measurement methods to understand the issues and phenomena truly. We are also working on the development of methods for this purpose.

Specifically, we are investigating multi-scale and multi-modal optical spectral imaging methods that combine microscopic photoluminescence and scanning electron microscopy-cathodoluminescence at different spatial scales for advanced compound and two-dimensional semiconductors. We are also working on ways that integrate scanning transmission electron microscopy images with three-dimensional atom probe methods.

2. Metrology informatics infrastructure

To efficiently advance research and development of materials and devices, the experimental cycle of measurement → design →synthesis/process must be effectively executed. For this purpose, a database that automatically accumulates experimental data is indispensable. Furthermore, the development of automated analysis techniques for measurement data is also required. For this purpose, we will work on technologies for automatic spectral data analysis, etc.



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Recent Research Papers and Achievements

1.Y. Yamaguchi, Y. Kanitani, Y. Kudo, J. Uzuhashi, T. Ohkubo, K. Hono, and S. Tomiya, “Atomic diffusion of Indium through threading dislocation in InGaN quantum wells” Nano Lett. 22, 6930-6935 (2022)

2. H. Yamamoto, K. Tanaka, S. Tomiya, S. Yamashita, M. Ukita, H. Nakano, R. Shirasawa, M. Kotera, K. Funatsu, “Dry Etching Damage and Alloy Composition Analysis of GaN-Based Semiconductors Using Electron Energy-Loss Spectroscopy” J. Elect. Matter 50, 4230 (2021)

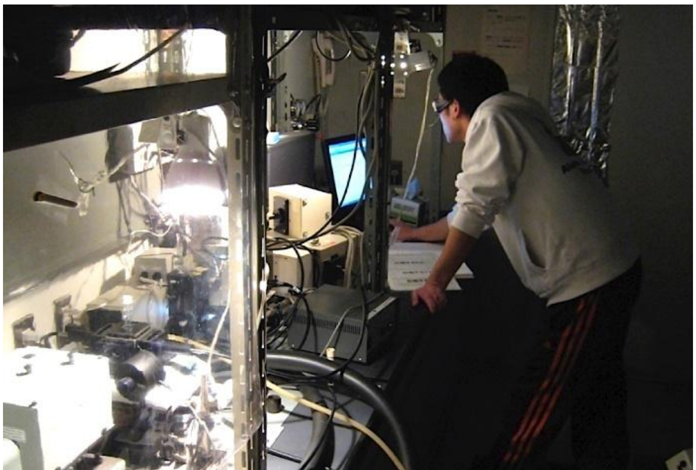
Research Environment

Having being selected by the Japanese government for numerous highly competitive funding programs since its creation, NAIST offers cutting-edge research facilities and environment both for master's and doctoral courses and for interdisciplinary research by highly motivated young researchers, with excellent support by specialized technicians.

Device Laboratory

Physics Laboratory

Chemistry Laboratory



Biomaterial Laboratory

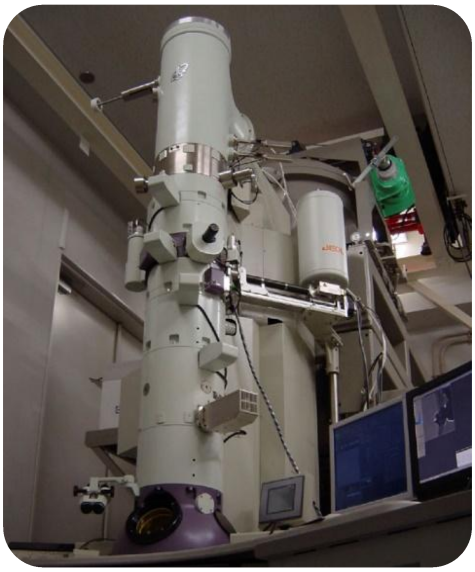
Campus-wide computer cluster

Research Environment

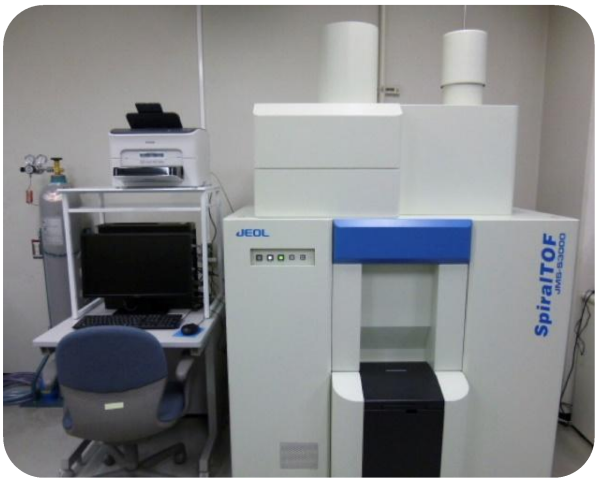
We offer cutting-edge experimental facilities and a spacious environment that allows all students to focus on their research and studies.

✓Various facilities cover wide fields in materials research.
✓ Over ten technical staffs are in charge of maintenance, user training an operation for users.
✓Web booking system and remote operation are available.
✓We are supported by MEXT-Program, “Advanced Research Infrastructure for Materials and Nanotechnology in Japan, ARIM”

X-ray Structure Analyzer



Transmission Electron Microscope (TEM)



MALD/SpiralTOF-MS

X-ray Photoelectron Spectroscopy

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Materials Science