

World Premier International Research Center Initiative (WPI)

FY 2024 WPI Project Progress Report (The center selected in and before FY2020)

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Research Center	Institute for Chemical Reaction Design and Discovery (ICReDD)		
Center Director	Satoshi Maeda	Administrative Director	Koichiro Ishimori

Common instructions:

- * Unless otherwise specified, prepare this report based on the current (31 March 2025) situation of your WPI center.
- * So as to execute this fiscal year's follow-up review on the "last" center project plan, prepare this report based on it.
- * Use yen (¥) when writing monetary amounts in the report. If an exchange rate is used to calculate the yen amount, give the rate.
- Prepare this report within 10-20 pages (excluding the appendices, and including Summary of State of WPI Center Project Progress (within 2 pages)).

Summary of State of WPI Center Project Progress (write within 2 pages)

1. Advancing Research of the Highest Global Level

To achieve sustainable development goals through the realization of Society 5.0, new chemical reactions are needed to create novel functional molecules and high-performance materials, and even medical treatments for intractable diseases. However, the design and discovery of new chemical reactions has relied on serendipity or experience-guided intuition, which has been a bottleneck in innovation for the new society. In the center, the computational research team, which is capable of simulating various types of chemical reactions, is engaged in the development of practical chemical reaction design techniques through close cooperation with information and experimental teams. To address various problems in highly complex chemical processes, the information team, which covers diverse fields ranging from chemical and materials informatics to combinatorial optimization, knowledge engineering, and mathematical modeling, was established by bringing together top information scientists in these fields. The experimental team also consists of top scientists from diverse backgrounds, such as organic synthesis, materials chemistry, polymer physics, and medical science. The center is engaged in developing "chemical reaction design and discovery" strategies for various application fields through high-level fusion research combining computational, informatics, and experimental techniques owned by these teams. Through these efforts, the center will revolutionize chemical reaction design and discovery. The achievements for FY2024 are as follows: 188 papers were published in peer-reviewed journals (39 papers in journals with an IF > 10). One paper was published in *Nature* (IF: 50.5), one in *Science* (IF: 44.8), and one in *Advanced Materials* (IF: 27.4), one in *Advanced Energy Materials* (IF: 24.4), and one in *Cell Host & Microbe* (IF: 20.6). The center members have presented their research in 68 invited lectures at international conferences and 17 awards have been granted. The total amount of research funding was 1,212 million JPY. Representative grants are JST-ERATO, JST-CREST, AMED-P-PROMOTE, etc.

2. Generating Fused Disciplines

Promotion of fusion research: The center was working on several flagship and bottom-up projects. These projects are evaluated yearly, and then, promising ones were expanded or promoted from bottom-up to flagship project. These projects were carried out under the Center Director's initiative with the Fusion Research Coordinator leading the project together with project leader.

Fusion research achievements in FY2024: There was progress in computation-informatics fusion research across multiple projects (*ACS Catal.*). The List group and Maeda group have made a significant breakthrough in organic chemistry by developing a novel method to activate alkanes (*Science*). Additionally, The Rubinstein group, Harabuchi (Fusion Research Coordinator), and Ito group have developed a theory that predicts the reaction rate of mechanochemical organic synthesis by using a ball mill. (*RSC Mechanochem.*). The Gong group, Takigawa group, Rubinstein group, and Tanaka group have developed a data-driven approach that integrates data mining, experimentation, and machine learning to design high-performance adhesive hydrogels from scratch, specifically tailored for demanding underwater environments (*Nature*).

Start-up support for fusion research: In FY2024, start-up support for new appointments (4.4 million yen for 4 new positions) and start-up support for fusion research to take on challenging bottom-up fusion projects (17 projects (17 million yen) and 1 group project (5 million yen) for a total of 22 million yen) were awarded.

Pre-checking system for the grant application: The center conducted a pre-checking system to review and revise the applications for Grants-in-Aid for Scientific Research, etc. before submission. 48% of the applications for Grants-in-Aid for Scientific Research were granted for FY2024 (university average 36.3%). The amounts of Grants-in-Aid for Scientific Research obtained have been increasing every year. FY2024: 333 million yen, and overseas PIs and Jr-PIs have also succeeded in

obtaining Grants-in-Aid for Scientific Research.

3. Realizing an International Research Environment

Number of researchers: The center conducted an international call for applications for new specially appointed faculty members and postdoctoral researchers to be hired at the center and received 122 applications for 15 positions from Japan and abroad in FY2024. As of March 31, 2025, the number of PIs was 15 including 3 foreign PIs, 41% of all researchers were foreign nationals, and 16% were female researchers (total of 79 researchers, including 32 foreign nationals and 13 female researchers, split between the fields of Computation the fields of Computation (16 researchers, 20%), Information (20 researchers, 25%), and Experiment (43 researchers, 55%).

Symposiums and seminars: The center has held the ICRéDD international symposium, inviting researchers from Japan and overseas to introduce them to the vision and research of the center. The 8th ICRéDD international symposium and the 2nd "Rising Star Program" by Junior PIs were jointly held on October 22-24, 2024. The symposium had 642 total participants (398 on-site/244 online), Total of 54 participants from overseas (15 countries), and 52 poster sessions. The 2nd "List Platform" Symposium was held on August 29th and had 78 participants. Furthermore, Hiroshima University SKCM² and ICRéDD held a joint international symposium on July 11. Both WPI centers presented their latest research, and 114 people (86 in person/28 online) attended the symposium. In FY2024, the center held 16 international seminars. Five co-organized symposiums, and two research ethics seminars were held in order to ensure opportunities for active communication.

Fostering young researchers by MANABIYA: Researchers were accepted through the MANABIYA system. "MANABIYA (ACADEMIC)" invited applications from March 2024 and accepted 24 researchers (7 were accepted from within Japan and 17 were accepted from abroad) out of 29 applicants, who were trained in the center's techniques.

4. Making Organizational Reforms

Evaluation system of center faculty members: FY2024. 3 faculty members received a two-level salary increase for evaluation grade S, 6 faculty members received a one-level salary increase for evaluation grade A, 2 faculty members received no revision salary for evaluation grade B, 2 faculty members received a one-level salary decrease for evaluation grade C and no faculty member received a two-level salary decrease for evaluation grade D. In FY2025, a new provision was established to provide postdoctoral fellows, for whom there had been no incentive system, to receive rewards for research papers with >10 IF.

Establishment of ICRéDD fellow system: In FY2024, two professors were appointed. The center provides ICRéDD fellows with our resources and we collaborate with them.

Strengthen the research support system: In FY2024, the DEI Promotion Team was established to develop measures to improve the gender balance of the center. The action plans were (i) to accelerate the increase of the proportion of female professors (inc. collaborators), (ii) to promote a limited open application for female faculty members and postdoctoral fellows, and (iii) to organize events for the project to support female junior and senior high school students in choosing careers in chemistry or information science in cooperation with the university office of the DEI.

5. Efforts to Secure the Center's Future Development over the Mid- to Long-term

The University has strongly supported the center and has secured funds equal to or more than the WPI grant for its operation (FY2024: 1,685 million yen). The university decided to make the center a permanent research center that would always promote cutting-edge, world-class research based on a new adaptive research strategy that would periodically change researchers and research topics and decided to allocate personnel costs equivalent to 13 professors. The "List-DX Catalyst Collaboration Research Platform (List-Platform)" and the "Mitsui Chemicals-ICReDD Innovative Chemical Reaction Design Laboratory (Mitsui Chemicals-ICReDD Laboratory)" functionally collaborated with the center. The university highly evaluates the center's achievements, such as a management system that clearly separates research and administrative organization, like a Center Director and Administrative Director, a careful performance evaluation system, a hospitality system, the assignment of faculty members specializing in fusion research (Fusion Research Coordinator), the development of measures to improve the gender balance of the center by DEI Promotion Team, instrument management faculty to prevent research misconduct, and ICRéDD fellow system.

6. Others

In FY 2024, an updated institutional annual report was created to convey the current direction of ICRéDD as well as monthly post card, quarterly news poster and newspaper, and MANABIYA pamphlet. A unique endeavor at the center is our quarterly news poster "The CATALYST". In FY2024, 3 issues were published in poster format: "Environmentally friendly reaction development: Force is the key? (Vol. 16)", "Designing crystals that spin (Vol. 17)", and "What is a reaction in the first place? (Vol. 18)". In addition, starting with the March 2025 issue, the magazine has been redesigned as "The Catalyst Newspaper" to focus on more familiar science topics in a newspaper style, with more pages and a larger circulation so that it can be read by more college and high school students. Novelty goods such as tote bags, satchels, file folders, pin badges, and stuffed toy keychains with ICRéDD branding were created. The center published 14 research-related articles on the web, including 8 research press releases and 6 research news articles. The center increased its public presence through a variety of other outreach events, such as a joint open campus event, a hands-on lab experience, a tour, a special class, and other activities.

- * Describe clearly and concisely the progress being made by the WPI center project from the viewpoints below.
- In addressing the below-listed 1-6 viewpoints, place emphasis on the following:
- (1) Whether research is being carried out at a top world-level (including whether research advances are being made by fusing disciplines).
 - (2) Whether a proactive effort continues to be made to establish itself as a "truly" world premier international research center.
 - (3) Whether a steadfast effort is being made to secure the center's future development over the mid- to long-term.

1. Advancing Research of the Highest Global Level

* Among the research results achieved by the center, concretely describe those that are at the world's highest level. In Appendix 1, list the center's research papers published in 2024.

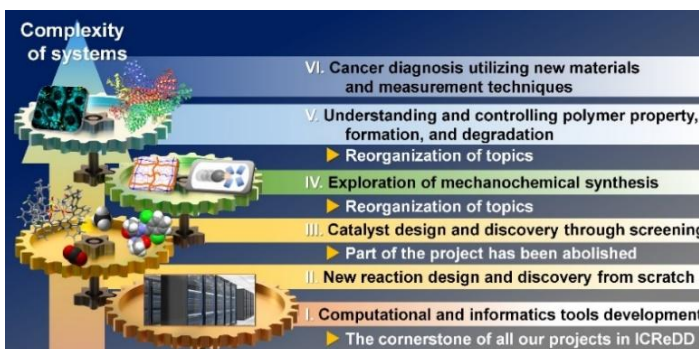
* Regarding the criteria used when evaluating the world level of center, note any updated results using your previous evaluation criteria and methods or any improvements you have made to those criteria and methods.

I. The center's scientific mission

To achieve sustainable development goals through the realization of Society 5.0, new chemical reactions are needed to create novel functional molecules and high-performance materials, and even medical treatments for intractable diseases. However, the design and discovery of new chemical reactions has relied on serendipity or experience-guided intuition, which has been a bottleneck in innovation for the new society. The center's mission is to establish "chemical reaction design and discovery" strategies and to enable humanity to purposefully design chemical reactions without relying on serendipity or experience-guided intuition. The center combines computational science, information science, and experimental science to develop new synthetic methods, new materials, and new applications in all areas of our society. In the center, the computational research team, which is capable of simulating various types of chemical reactions, is engaged in the development of practical chemical reaction design techniques through close cooperation with information and experimental teams. To address various problems in highly complex chemical processes, the information team, which covers diverse fields ranging from chemical and materials informatics to combinatorial optimization, knowledge engineering, and mathematical modeling, was established by bringing together top information scientists in these fields. The experimental team also consists of top scientists from diverse backgrounds, such as organic synthesis, materials chemistry, polymer physics, and medical science. In the center, we are engaged in developing "chemical reaction design and discovery" strategies for various application fields through high-level fusion research combining computational, informatics, and experimental techniques developed by these teams. Through these efforts, the center will revolutionize chemical reaction design and discovery.

II. Overview of the center's research

In FY2024, we decided to continue six flagship projects which were decided by the internal evaluation held at the end of FY2021. Among them, Project I is the most important project in ICReDD. It is closely related to all the other projects and provides computational acceleration tools for them. During monthly meetings, all computational and informatics groups come together to share successes and failures based on their contributions to the other flagship projects. This feedback loop allows us to stay abreast of the latest state-of-the-art computational and informatics tools being used in these projects and helps us to further develop these tools. The other projects have a hierarchical complexity. The complexity increases in the order of the project number. In other words, the number of atoms involved in the reaction treated in each project increases in that order. Working simultaneously on these projects of varying complexity will allow us to build a comprehensive set of tools that can be applied to a wide range of problems in the chemical and materials sciences.



The list of these projects is shown below:

Project-I: Computational and informatics tools development. We consistently make Project I the cornerstone of all our projects. All computational and informatics PIs work with Project I and provide feedback on the application of their tools to other projects. This feedback loop strengthens our foundation and helps accelerate all of our projects. The goal of this project is to create a set of *in silico* reaction design strategies that can be tailored to individual cases. In the first half of the WPI period, Project I contributed to the development of the QCaRA/AFIR approach, which

combines the AFIR method with a graph-theory-based method for calculating reaction yields, leading to the first-principle discovery of previously unexplored chemical reactions. In addition, a cheminformatics-based approach to predicting the enantioselectivity of organocatalysis has contributed to the discovery of new catalysis. Two goals for the second half of the WPI period are the development of a method for designing an appropriate organometallic catalyst for a given chemical transformation (related to Project II) and the design of a high performance organocatalyst that achieves asymmetric activation of unfunctionalized molecules (related to Project III).

Project-II: New reaction design and discovery from scratch. We continue to work on a project to predict new reactions from scratch using reaction path networks based on quantum chemical calculations (former Project II). So far, we have demonstrated several successful examples of (non-catalytic) small molecule synthesis. In the future, we will focus our efforts on the discovery of catalysis. This can be done in part on the basis of the achievements in non-catalytic reactions made in the first half of the WPI period, but is a much more complex matter requiring the further development of computational and informatics tools. The goal of this project is to establish a systematic design framework for discovering an organometallic catalyst that can achieve previously unexplored chemical transformations.

Project-III: Catalyst design and discovery through screening. Project III replaces the Supramolecular Catalytic Reaction Space Design project (former Project III) that we were working on. In its current form, the project involves finding the optimal substituents for certain transformations in molecular catalysts. For example, we aim to improve the enantioselectivity of List's IDPi catalyst for various chemical transformations by using a computational and informatics-based approach to screen and optimize the substituents of the catalyst. The goal of this project is to achieve an asymmetric activation of unfunctionalized molecules with the assistance of a computational and informatics approach. Such a transformation is highly difficult to achieve by an organocatalyst and is an appropriate target for the second half of the WPI period.

Project-IV: Exploration of mechanochemical synthesis. Project IV is related to the Bridging Micro- and Macro-World project (former Project IV), but focuses exclusively on mechanochemical synthesis using ball mills. It is an ideal target for our computational and informatics tools because of its rapidly growing importance and the large amount of unexplored knowledge that remains. This synthetic method has proven to be a promising tool in organic synthesis. However, its applicability and understanding have not yet been sufficiently explored. The goal of this project is to expand its applicability, elucidate unexpected species unique to this synthesis, and construct a theory for modeling the effects of mechanical impact. Based on the rational design of mechanochemical reactions we will investigate target reactions such as the cross-coupling of solid materials, synthesis of new organometallic reagents like Grignard reagents in the solid state, and the decomposition and recycling of polymer materials.

Project-V: Understanding and controlling polymer property, formation, and degradation. Project V is an extension of the Polymer Degradation Project (former Project VI) that we have been working on. The project, in its current form, involves the design of polymer properties through simulation, the visualization of polymer mechanoradicals, the exploitation of polymer mechanoradicals, the design of polymer sequences to maximize desired properties, and more. Two goals of this project are to improve the performance of muscle-like double network hydrogels and to utilize plastic materials in the synthesis of useful materials.

Project-VI: Cancer diagnosis utilizing new materials and measurement techniques. We will continue our work on developing cancer diagnostic methods using new materials and measurement techniques (former Project VII). In particular, we will further investigate the hydrogel-activated reprogramming phenomenon (HARP) that was discovered during the first half of the WPI period. Two goals of this project are to understand HARP properly and to achieve its clinical applications by a fusion team of materials scientists, information scientists, and medical scientists.

In addition, in partnership with the School of Medical Science, we have launched a consortium called the Clinical Platform for Chemical Reaction Collaboration. Through this consortium, we aim to accelerate the use of our chemical products in medical diagnosis and treatment.

Bottom-up projects: Furthermore, we have provided opportunities for young researchers to propose new ideas and launch related bottom-up projects. The launch of each bottom-up project is supported by an internal budget called Fusion Research Start-up. Based on their results, successful bottom-up projects are promoted as flagship projects, while underperforming flagship projects are evaluated and may be discontinued. This approach allows us to consistently deliver high-impact results while encouraging the activities of our young researchers.

III. Achievements and progress on the center research

Below, preliminary reports and interdisciplinary collaborations are marked as follows.

* Preliminary report (confidential)

† Interdisciplinary collaboration within the center

‡ Interdisciplinary collaboration with groups outside the center

Below, achievements and progress on the above flagship and bottom-up projects are showcased.

1) Achievements and progress on the Project-I: Computational and informatics tools development

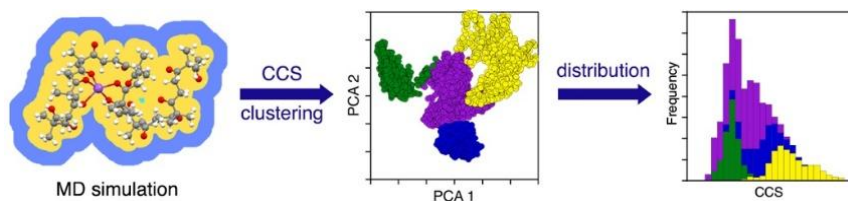
The development and integration of fundamental computational and informatics methods are key issues in developing strategies for computational and informatics driven chemical reaction design and discovery. In FY2024, the achievements and progress are on three topics: a neural network potential-based AFIR (NNP/AFIR)-based design of thermally stable mechanophore (**1-1**), an MD-based CCS simulation method (**1-2**), and an end-to-end tool for designing retrosynthetic routes (**1-3**).

*†1-1) NNP/AFIR-based design of thermally stable mechanophore for self-strengthening materials

The **Gong group**, **Maeda group**, **Varnek group**, and **Jiang group** have developed a general selection rule to identify force-sensitive molecules and employed it to discover mechano-reactive molecules that could be employed in the self-strengthening materials. Normally, a conventional mechanophore has either weak covalent bonds or strained rings, leading to its thermal and UV instability. To find a novel mechanophore that only reacts under force stimuli remains as a challenge in this field. Here, based on our experiences in mechanochemistry, we believe a special conformational motif called "node" can promote the force effect significantly. Subsequently, the Extended-AFIR (EX-AFIR) method was utilized to render the activation force levels of two natural products which have the "node" motif. These two compounds, camphanediol and pinanediol, were used as the auxiliary ligands in the asymmetric synthesis and never thought to be mechano-reactive. However, to be a qualified mechanophore used in the self-strengthening material, a low F_{act} is a necessary but hardly sufficient condition. In fact, to trigger the following polymerization reaction with monomer fed into the system, a relatively long-lived mechanoradical is required. To test all the possible pathways that the mechanoradical may undergo, a reaction network exploration was realized by the EX-AFIR/NNP method developed by the **Varnek group**. This machine-learning method allows a rapid exploration with a considerably accurate energy output and small computational cost. The calculations indicated that camphanediol would generate relatively stable radical while pinanediol would end up with two alkene molecules. Finally, a hydrogel with camphanediol was prepared and tested by the **Gong group**. Owing to the selection rule, this material showed satisfactory performance of self-strengthening but with strong thermal and UV stability. This is significant progress compared to our previous azo-based material (*Chem. Sci.* 2025).

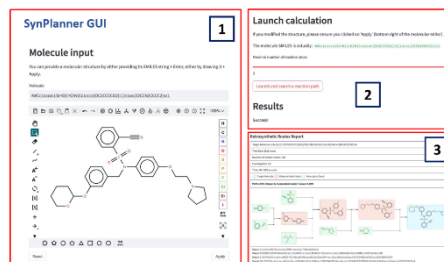
†1-2) MD-based CCS simulation method

The **Taketsugu group** and **Inokuma group** have developed a molecular dynamics (MD) based conformational search method for simulating collision cross section (CCS) distributions that can be obtained from experimental ion mobility-mass spectrometry (IM-MS). As a case study, the gas-phase conformations of discrete polyketones composed of the 3,3-dimethylpentane-2,4-dione repeating unit were analyzed. These polyketones have recently been developed in **Inokuma group** as structurally flexible molecular components for derivatization to π -conjugated chromophores, metal ion adsorbents, lithium-ion conductors, and cation/anion binding macrocyclic hosts. Conformational analysis of the cation binding states is important for designing and fine tuning their molecular functions. The conformational simulation method demonstrated qualitative reproduction of the arrival time distributions observed by IM-MS. Furthermore, the clustering analysis of the MD-simulated structures clarified the correspondence between CCS distribution and structural character (*Adv. Theory Simul.* 2024).



*†1-3) Building up the GUI for SynPlanner

The **Varnek group** has developed SynPlanner - an end-to-end tool for designing customized retrosynthetic planning from reaction data (*J. Chem. Inf. Model.* 2025). It includes a reaction data curation pipeline, reaction rule extraction, retrosynthetic model training, and retrosynthetic planning. The tool supports the customization of each step of the pipeline to address different needs in the development of customized retrosynthetic planning solutions. The retrosynthetic planning is performed by Monte-Carlo Tree Search guided by graph neural networks for retrosynthetic rules prediction and precursors synthesizability prediction. A Graphical User Interface (GUI) allows users (1) to input a target molecule either in SMILES format or to draw its structure manually with the help of a chemical structure editor, (2) to specify the maximum number of steps of the retrosynthetic route, and (3) to visualize the found retrosynthetic routes. For each target molecule, SynPlanner can generate dozens of plausible retrosynthetic routes. To assess their feasibility, we sought to integrate human expertise in the modeling workflow. For an ensemble of reaction routes generated with the tool, a chemist can assess synthetic feasibility of their individual steps. These assessments can be used to train a machine learning model to estimate the feasibility of SynPlanner solutions for any new target molecule.

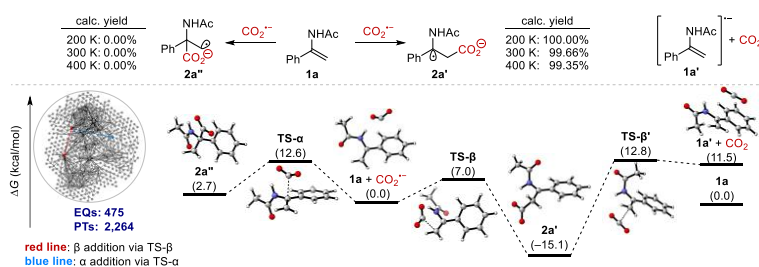


2) Achievements and progress on Project-II: New reaction design and discovery from scratch

We continue to utilize reaction path networks calculated by AFIR to realize small molecule activation reactions. In FY2024, electrochemical and photochemical approaches for the synthesis of β -amino acids by incorporating CO₂ (**2-1**) and Virtual Ligand-Assisted Optimization (VLAO) (**2-2**) were achieved.

†2-1) Photoredox catalyzed radical reaction based on CO₂

The **Mita group** and **Maeda group** have developed a novel approach utilizing the CO₂ radical anion as a key intermediate for the synthesis of β -amino acids from *N*-Ac-enamides. Both electrochemical and photochemical techniques were employed to generate the CO₂ radical anion under mild

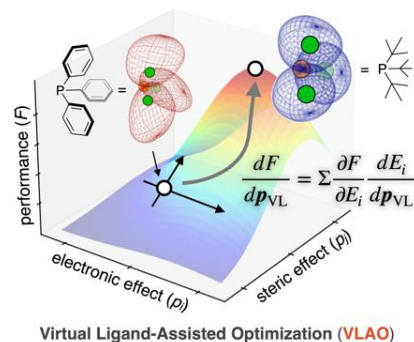


conditions. The feasibility of the synthesis of β -amino acids was confirmed through an automated reaction path search using the AFIR method. This work highlights the potential of CO₂ as a versatile building block in organic synthesis and provides a sustainable alternative to conventional methods for producing β -amino acids (*ChemistryEurope* 2025). Another collaborative work also discloses an elegant synthetic route to β -amino acids via the direct addition of an aminium radical, generated through the one-electron oxidation of a secondary amine, to alkenes, followed by trapping with CO₂. The successful development of a synthetic route to β -amino acids from CO₂ was achieved by employing computational chemistry, namely the Energy shift (ES)/AFIR method, as an efficient prediction tool. By using an Ir-based photoredox catalyst and irradiation with blue LED light, high yields of several β -amino acids were obtained as expected (*ACS Catal.* 2025).

†2-2) Virtual Ligand-Assisted Optimization (VLAO)

The **Maeda group** and **Iwata group** have developed a technique called Virtual Ligand-Assisted Optimization, or VLAO, to streamline the design of ligands, which are important molecules in transition metal catalysis. Historically, this process has been guided by ligand descriptors such as Tolman's electronic parameter and the cone angle. Analyzing reaction outcomes in terms of these parameters has enabled chemists to identify the most important properties for controlling catalytic activities. However, typical strategies for these analyses rely on regression approaches, which often require extensive experimental studies to identify trends across chemical space. The groups

introduced the VLAO method, a computational approach for reactivity-directed ligand engineering. This method utilizes the virtual ligand (VL), a mathematically modeled entity for quantum chemical calculations designed to approximate electronic and steric properties of phosphine ligands. Whereas the electronic and steric parameters of a real ligand are inherently determined by its chemical structure, those of a VL can be independently tuned. The VLAO method exploits this feature of VLs to analyze a reaction outcome. The responses of a reaction outcome to changes in the electronic and steric parameters are quantified by calculating the differentiation. The introduction of such analytical gradients facilitated numerical optimization of the ligand properties. The obtained optimal parameters can be used as a rational guideline for designing optimal real ligands. The VLAO method was computationally validated in the optimization of monodentate and bidentate phosphine ligands including asymmetric ligands. In addition, the utility of the VLAO method was experimentally demonstrated in the α -selective hydrogermylation of a terminal ynamide (*ACS Catal.* 2024).

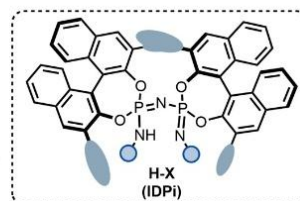
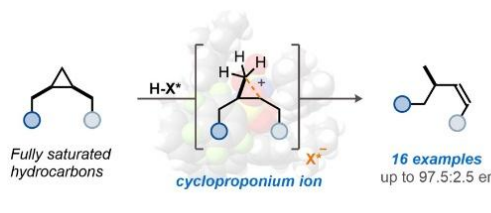


(3) Achievements and progress on Project-III: Catalyst design and discovery through screening

Project III involves finding the optimal substituents and conditions for catalysts through a computational screening process. In FY2024, we made a significant achievement in developing a method for stereoselective activation of alkanes (**3-1**) and the integration of the DOPTools automated library with the CADS platform (**3-2**).

*†3-1) Asymmetric fragmentation of cyclopropanes

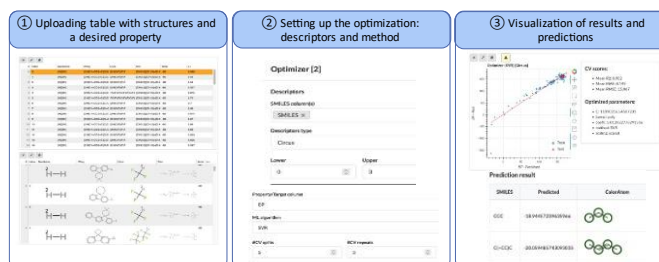
The **List group** and **Maeda group** have made a significant breakthrough in organic chemistry by developing a novel method to activate alkanes, compounds that are crucial in the chemical industry. The stereoselective activation of



alkanes constitutes a long-standing and grand challenge for chemistry. Although metal-containing enzymes oxidize alkanes with remarkable ease and selectivity, chemical approaches have largely been limited to transition metal-based catalytic carbon-hydrogen functionalizations. Alkanes can be protonated to form pentacoordinated carbonium ions and fragmented into smaller hydrocarbons in the presence of strong Brønsted acids. However, catalytic stereocontrol over such reactions has not previously been accomplished. We show here that strong and confined acids catalyze highly enantioselective fragmentations of a variety of cyclopropanes into the corresponding alkenes, expanding the boundaries of catalytic selective alkane activation. Computational studies suggest the involvement of the long-debated cyclopropanium ions (*Science* 2024).

*†3-2) Development of DOPTools and its implementation to CADS platform

The **Sidorov group**, **Takahashi group**, and **List group** have developed a web-based application for optimization of predictive machine learning (ML) models. While ML is a powerful tool for reducing the experimental load by filtering out the compounds and reactions that would not potentially lead to desired results, most algorithms require extensive optimization for better performance. The **Sidorov group** has developed DOPTools (*Digital Discovery* 2025), a library that performs the benchmarks of molecular descriptors and ML methods in an automated manner via a command-line interface for any desired property. Together with **Takahashi group**, they have also created a web-based platform that allows for easy access to the functionality of the



DOTools library, based on the CADS platform. This platform allows the user to submit their data with chemical structures and the desired property to the server, choose the descriptor type and an algorithm to be optimized, and the server will perform the optimization without any further intervention from the user. Afterward, the best models can be saved and used to predict external data and to interpret the modeling results via ColorAtom methodology.

4) Achievements and progress on the Project-IV: Exploration of mechanochemical synthesis

Ball mill-based mechanochemical synthesis has emerged as a promising tool in organic synthesis. However, despite its growing importance, little is understood about this new method. In FY2024, we developed novel synthetic strategies related to ball mill synthesis (4-1) and a theory that predicts the reaction rates of organic mechanochemical reactions using a ball mill (4-2).

†4-1) Mechanochemical synthesis with the ball mill technique

The **Ito group** and **Maeda group** have achieved a mechanochemical strategy based on ball-milling that facilitates the direct generation of various aryl lithium nucleophiles from commercially available unactivated barium metal and aryl halides without complicated pre-activation processes. Organobarium reagents are of interest as homologues of the Grignard reagents based on organomagnesium compounds due to their unique reactivity as well as regio- and stereoselectivity. However, reactions involving organobarium reagents are less developed in comparison to reactions involving Grignard reagents due to the lack of a simple and economical synthetic method and their high reactivity. The simple mechanochemical protocol allows the rapid development of novel carbon–silicon-bond-forming reactions with hydrosilanes mediated by aryl barium nucleophiles; importantly, these reactions are difficult to achieve using other Grignard-type carbon nucleophiles. The reaction mechanism of the hydrosilane arylation were elucidated computationally by the **Maeda group** using the artificial force-induced reaction (AFIR) method (*Chem. Sci.* 2024).

Furthermore, the **Ito group** has developed a mechanochemical method for the direct generation of organolithium reagents from readily available organic halides and unactivated lithium metal (lithium wire) under bulk-solvent-free conditions. Organolithium species are excellent precursors for generating new carbon–carbon and other carbon–heteroatom bonds, however, they are typically air, moisture, and temperature sensitive. These reactions rapidly generate a diverse array of organolithium compounds at room temperature without special precautions against moisture and without temperature control. The addition of these compounds to various electrophiles proceeds smoothly in a one-pot fashion. This approach enables reactions with poorly soluble aryl halides and direct C–F bond lithiation that are inefficient under conventional solution-based conditions (*Nature Synth.* 2025).



†4-2) Scaling theory for the kinetics of mechanochemical reactions with convective flow

The **Rubinstein group**, **Harabuchi (Fusion Research Coordinator)**, and **Ito group** have developed a theory that predicts the reaction rate of mechanochemical organic synthesis by using a ball mill. The mechanochemical reactions between solid reactants occur at their interface. The new theory predicts that and create a distinct interfacial phase rich in product and the dissolution of reactant molecules into this phase governs the reaction rate. A small volume of solvent added to the system can act as a plasticizer of the product-rich phase. Our theory predicts that the mechanical stress applied by the balls drives plastic flow in the product rich phase and this accelerates the mechanochemical reactions (*RSC Mechanochem.* 2024). Compared to conventional organic synthesis, the theoretical foundation of mechanochemical organic synthesis is still in its infancy. Bridging this mesoscopic theory and microscopic quantum chemical calculations developed by **Maeda group** will guide the design of mechanochemical organic synthesis.

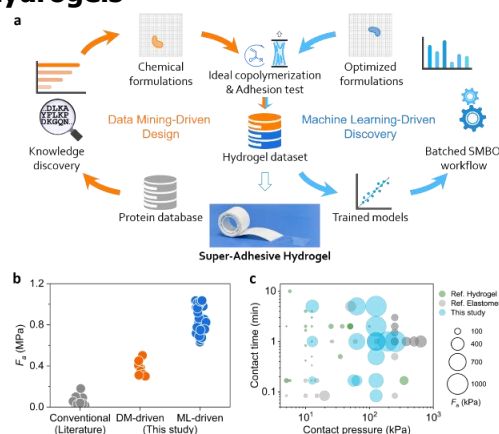
(5) Achievements and progress on the Project-V: Understanding and controlling polymer property, formation, and degradation

This project includes the design of polymers to exhibit unique properties, machine learning, the

use of polymer mechanoradicals, and the control of polymer network structures to maximize desired properties. In FY2024, we had progress in designing underwater functional adhesive hydrogels (**5-1**), achieving rapid self-strengthening hydrogels utilizing force-sensitive molecules (**5-2**).

*†5-1) Sequence-controlled underwater adhesive hydrogels

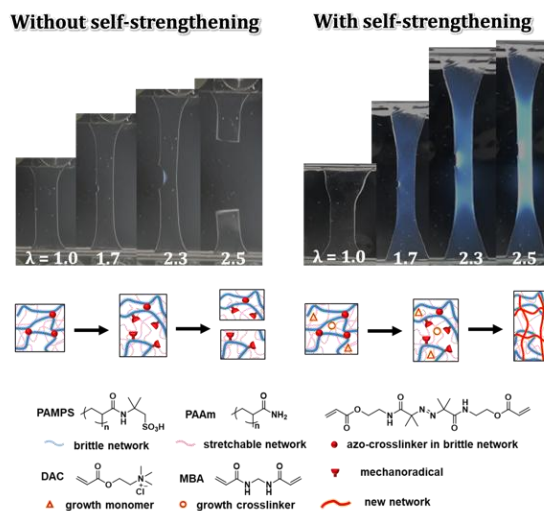
The **Gong group**, **Takigawa group**, **Rubinstein group**, and **Tanaka group** have developed a data-driven approach that integrates data mining, experimentation, and machine learning to design high-performance adhesive hydrogels from scratch, specifically tailored for demanding underwater environments. By leveraging protein databases, they devised a descriptor strategy to statistically replicate protein sequence patterns in polymer strands through ideal random copolymerization, enabling targeted hydrogel design and dataset construction. Using machine learning, they optimized hydrogel formulations from an initial dataset of 180 bioinspired hydrogels, achieving a remarkable improvement in adhesive strength, with a maximum value exceeding 1 MPa. These super-adhesive hydrogels hold immense potential for applications ranging from biomedical engineering to deep-sea exploration.



Data-driven methodologies have successfully advanced the discovery and prediction of hard materials with well-defined atomic structures by utilizing standardized datasets, accurately predicting properties, and efficiently exploring the design space. However, applying these methodologies to soft materials has remained a significant challenge due to their inherently complex and multiscale structure–property relationships. This study establishes a concrete approach for extending data-driven methodologies to soft materials, marking a major breakthrough in the field (*Nature* 2025).

*†5-2) A rapid self-strengthening mechanism in double-network hydrogel

The **Gong group** and **Rubinstein group** have developed a rapid self-strengthening mechanism in double-network hydrogel that is activated upon deformation of the material. This was accomplished by installing weak chemical bonds as sacrificial bonds into the first network. Upon deformation of the material, these weak sacrificial bonds break and trigger mechanochemical reactions, forming new networks rapidly enough to reinforce the material during deformation and significantly improve crack resistance. This rapid strengthening exhibits strong rate dependence, dictated by the interplay between mechanoradical-related bond breaking and the kinetics of mechanoradical-initiated polymerization of monomers to form new networks. As such network formation is generally applicable to diverse monomers and crosslinkers with different kinetics, a wide range of mechanical properties can be obtained. These findings may inspire the design of tough polymer materials with on-demand, rate-dependent mechanical behaviors through mechanochemistry, broadening their applications across various fields (*Nat. Mater.* 2025).



(6) Achievements and progress on the Project-VI: Cancer diagnosis utilizing new materials and measurement techniques

We have continued to investigate HARP, which was discovered during the first half of the WPI period. Understanding HARP and its potential clinical applications are pressing issues to be addressed in this project. In FY2024, we discovered that leukemic cells cultured on synthetic polymer hydrogels acquired the properties of leukemia stem cells (LSCs), which shifted the metabolic state to OXPHOS (**6-1**). We also developed a system that uses artificial intelligence to enable accurate

Raman spectroscopy measurement that could be useful in discriminating cancer stem cells (CSCs) from differentiated cancer cells (6-2).

*6-1) Application of the HARP phenomenon to leukemia cells and the effect of the stiffness of the tumor microenvironment on HARP

The **Tanaka group** and **Gong group** previously reported the rapid reprogramming of cancer cells to cancer stem cells (CSCs) using hydrogels, which was named the hydrogel activated reprogramming (HARP) phenomenon. It is an urgent task to apply this technology clinically, understand the properties of each CSCs, and identify new therapeutic target molecules to eradicate them. In FY2024, we discovered that leukemic cells cultured on synthetic polymer hydrogels acquired the properties of leukemia stem cells (LSCs), which shifted the metabolic state to OXPHOS. In hydrogel-generated LSCs, single-cell RNA sequencing identified the increase in expression levels of AKR1B1 and TSPYL5 that play an essential role for stemness generation, which may become therapeutic targets for LSCs (*Biochem. Biophys. Res. Commun.* 744:151149, 2025).

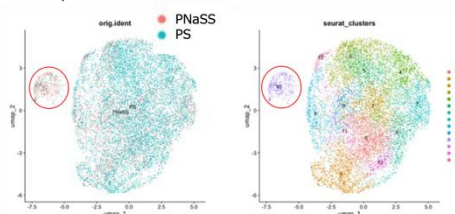
On the other hand, to elucidate molecular mechanisms underlying CSCs generation, we focused on the elastic modulus of hydrogels mimicking the stiffness of tumor tissues. The H-Ras-, but not Src-, transformed mouse NIH3T3 fibroblasts induced stem cell properties on the PAMPS gel, particularly with elastic modulus of approximately 10 kPa that mimics general tumor tissues. Ca²⁺ channels such as *TRPC* and *TRPV* families were also upregulated on the gel with 10 kPa. These findings suggest that tumor tissues with a stiffness of 10 kPa effectively trigger the signals for generating CSCs through alterations of membrane structures and Ca²⁺ influx, which will be beneficial for developing novel therapeutic applications targeting CSCs (*Biochem. Biophys. Res. Commun.* 743:151163, 2025).

In parallel with the above studies, the **Tanaka group** and **Gong group** investigated the effects of hydrogels on normal tissue stem cells, leading to the discovery that culture on certain hydrogels induces reprogramming of adult intestinal cells into the fetal intestine-like state characterized by unique fetal-like gene expression profiles, spheroid-forming ability, and growth factor independence. Given that some colorectal cancer (CRC) cells acquire fetal-like properties during development, we examined if hydrogel culture could recapitulate this fetal reprogramming in CRC cells. The results revealed that synthetic hydrogels simultaneously induce intestinal stem cell and fetal cell signatures, recapitulating fetal-like CRC stem cells with high tumorigenic ability and drug resistance. This hydrogel-induced reprogramming of CRC cells was mediated by the activation of the Src-Yap and Src-Erk5 signaling pathways. Finally, a mouse model of fetal-like CRCs has been developed for future examination of anti-cancer drug candidates (*BMC Cancer* 25:405, 2025). These findings demonstrate the usefulness of synthetic hydrogels in recapitulating fetal-like cancer cells, a novel type of CSCs in CRC, potentially aiding development of effective therapies against CRCs with fetal-like properties.

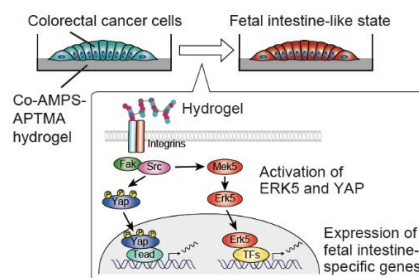
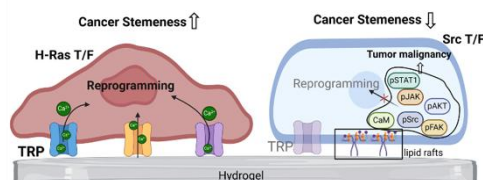
6-2) Development of a system that uses artificial intelligence to enable accurate Raman spectroscopy measurement

Spontaneous Raman microscopy offers label-free, rich chemical information but suffers from long acquisition time due to extremely small scattering cross-sections. The **Komatsuzaki group** developed a new Raman microscope combined with artificial intelligence called multi-armed bandits algorithm, in which by exploiting the information acquired on the fly, experimental conditions can be "optimized" while exploring previously unseen parts of the sample. In addition, the accuracy of measurements can be guaranteed mathematically by defining an objective of the measurement,

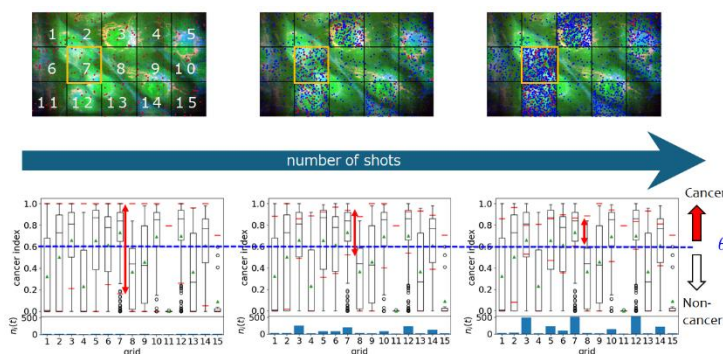
Leukemia cells cultured on PNaSS gel were allocated to cluster 10, and expression levels of AKR1B1 and TSPYL5 were increased.



The influence of oncogenes such as H-Ras and Src in cancer stemness induction dependent on the stiffness of the tumor microenvironment.



such as a diagnosis. This microscope technique requires 3,333 to 31,683 times smaller number of illuminations for discriminating cell phenotypes of follicular thyroid carcinoma than conventional scanning, by reflecting the underlying Raman fingerprints, potentially aiding development to discriminate CSCs and differentiated cancer cells studied in **Gong group** and **Tanaka group** (*PNAS* 121: e2304866121, 2024).

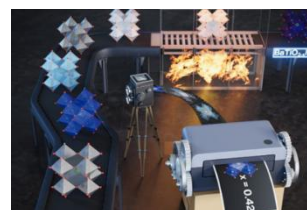


(7) Achievements and progress on Bottom-up projects

Bottom-up projects are initiatives led mostly by our young researchers, and five outstanding projects from FY2024 are highlighted below. The machine-learning (ML) models for evaluating chemical composition from images were expanded (**7-1**). The selective mono-hydrodefluorination of trifluoromethylarenes was designed (**7-2**). A copper-catalyzed N-arylation methodology for the efficient conversion of indigo dye into functional red-light photoswitches was achieved (**7-3**). Novel pH-responsive dyes for cancer cell photoacoustic imaging were developed (**7-4**). Finally, the photoinduced charge transfer emission from 4f- to π -orbitals using a trivalent europium (Eu(III)) complex was achieved (**7-5**).

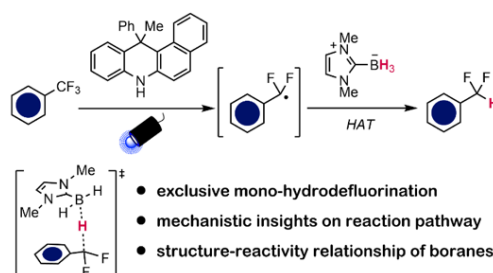
†7-1) Prediction of Perovskite Oxyhydrides using image-based machine learning system

The **Inokuma group** and **Takigawa group** have developed an efficient image-based ML system for rapid and accurate prediction of hydride content in perovskite oxyhydride ($\text{BaTiO}_{3-x}\text{H}_x$). Hydride content in perovskite oxyhydrides represents a crucial parameter that governs the properties of the materials. However, the synthesis of the oxyhydrides with precise control over the hydride content x remains a challenging task. Photographs of powder samples with experimentally determined hydride contents were used to develop the ML training data set that can analyze samples with unknown hydride contents using an ExtraTrees algorithm. Using this ML system, detailed profiles of thermal hydrogen release of $\text{BaTiO}_{3-x}\text{H}_x$ were quantitatively analyzed to demonstrate the feasibility of fine-tuning the hydride content within $0 \leq x \leq 0.4$ by adjusting the processing temperature. These results demonstrate an application of image-based ML for the fine-tuning of oxyhydride materials (*ACS Appl. Eng. Mater.* 2024).



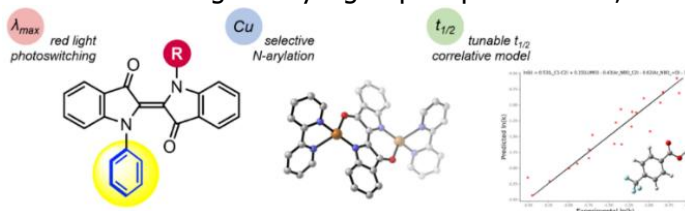
†7-2) Photocatalytic mono-hydrodefluorination of trifluoromethylarenes using *N*-heterocyclic carbene borane via hydrogen atom transfer

The **Huang group** and **Maeda group** have achieved selective mono-hydrodefluorination of trifluoromethylarenes (ArCF_3) using *N*-heterocyclic carbene boranes (NHC-BH_3) as the hydrogen atom transfer (HAT) reagent. HAT is a fundamental mechanism in radical reactions. Photoexcitation of a recently reported photocatalyst under blue LED irradiation enables the selective reduction of ArCF_3 to generate ArCF_2^\bullet radical species. Subsequent HAT between NHC-BH_3 and this radical intermediate affords the desired product. Detailed experimental and computational studies provided substantial evidence for the proposed HAT mechanistic pathway. Notably, computation and data science approaches allowed us to build a classification model based on readily obtainable molecular descriptors to explain the reactivity differences across a selection of boranes. Our synthetic method gives access to new CF_2H -containing compounds and is applicable to ArCF_3 bearing attractive motifs such as amino acids and carbohydrates. Overall, this study provides in-depth mechanistic and quantitative understandings of boryl radical chemistry with relevance to hydrodefluorination reactions (*ACS Catal.* 2024).



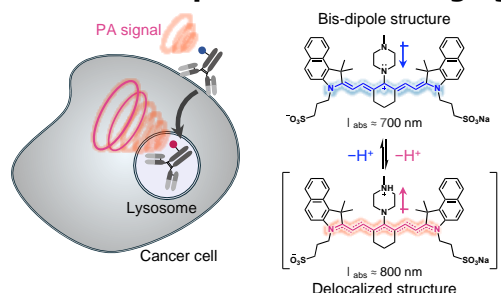
†7-3) Accessing a Diverse Set of Functional Red-Light Photoswitches by Selective Copper-Catalyzed Indigo *N*-Arylation

The **Huang group** and **Maeda group** have developed a copper-catalyzed *N*-arylation to efficiently convert indigo dye into functional red-light photoswitches. Photoswitches have emerged as a crucial component in photo-responsive systems with wide applications in the fields of biomedical and materials science. The installation of indigo *N*-aryl groups containing synthetically useful functional motifs was achieved for the first time, an important step towards their real applications. The surprising selectivity for mono-*N*-arylation is explained by theoretical calculations, where a key bis-copper-indigo intermediate is proposed to lower the energy barrier of the most challenging step. Furthermore, through a data-science workflow involving *N*-aryl group representation, DFT featurization, and multivariate linear regression, models correlating the thermal half-lives and structures of these indigo photoswitches were constructed, which is expected to aid future rational design of this attractive class of compounds (*J. Am. Chem. Soc.* 2024).



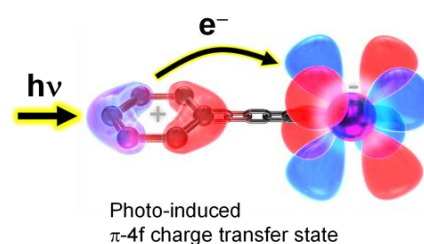
†7-4) Development of pH-responsive Cy7.5 dyes for cancer cell photoacoustic imaging

The **Ogawa group** and **Taketsugu group** have developed novel pH-responsive Cy7.5 dyes for cancer cell photoacoustic (PA) imaging. Among various Cy7.5 derivatives, pH-dependent absorption spectral changes were observed for derivatives with a diazaalkyl group such as piperazine. DFT calculations and absorbance measurements showed these changes depended on the electron density of the N atom at position 4 of piperazine. The PA spectra also varied with pH. In PA imaging with cancer cells, the pH-responsive dyes conjugated to a cancer specific antibody accumulated in cancer cells and changed their PA signals in response to the acidic lysosomal pH. These findings highlight the potential of pH-responsive Cy7.5 dyes for cancer detection, and the elucidated mechanism of the spectral change could contribute to designing new PA imaging agents (*J. Photochem. Photobiol. A: Chem.* 2024).



†7-5) Photoinduced charge transfer (CT) emission from 4f- to π -orbitals

The **Hasegawa group** and **Taketsugu group** have achieved the photoinduced charge transfer (CT) emission from 4f- to π -orbitals using a trivalent europium (Eu(III)) complex, supported by both experimental and theoretical analyses. The Eu(III) complex exhibits an eight-coordination structure, comprising three anionic nitrates and two neutral electron-donating ligands containing a carbazole unit. The diffuse reflectance spectrum of the complex displays an absorption band at 440 nm and time-resolved emission analyses reveal a characteristic emission band at 550 nm. Comparative studies employing a trivalent gadolinium (Gd(III)) complex, alongside quantum chemical analyses, confirm that the observed absorption and emission bands are associated with CT transitions between π - and 4f-orbitals. The observation of CT emission based on the 4f-orbital offers novel insights into the field of molecular luminescence science and technology (*Commun. Chem.* 2025).



2. Generating Fused Disciplines

* Describe the content of measures taken by the center to advance research by fusing disciplines. For example, measures that facilitate doing joint research by researchers in differing fields. If any, describe the interdisciplinary research/fused discipline that have resulted from your efforts to generate fused disciplines. You may refer to the research results described concretely in "1. Advancing Research of the Highest Global Level."

Promotion of fusion research: The center is working on several flagship projects. Each project

involves groups from two or more disciplines. Setting and working on such flagship projects together has been a strong driving force to promote interdisciplinary fusion in the center. In addition, the center holds a call for ideas from mainly young researchers in the center and provides them with an opportunity to lead a bottom-up project. These flagship and bottom-up projects are evaluated yearly. Then, promising ones are expanded or promoted from bottom-up to flagship projects. Conversely, ones that are not proceeding well are terminated or restarted as a bottom-up project. These projects are carried out under the Center Director's initiative. To do that, "Fusion Research Coordinator" join periodic meetings of all these projects and report their progress to the Center Director. Additionally, the Fusion Research Coordinator participates as a computational scientist in a project themselves and leads the project together with the project's leader. In FY2024, all PIs, junior PIs, and Co-PIs had an opportunity to discuss each topic of flagship and bottom-up projects at monthly PI meetings to open up research in the center. Periodical social gathering events, so-called "ICReDD get togethers" were held 6 times, where young researchers, students and PIs communicated and exchanged their opinions. As for start-up support, the Director and the Fusion Research Coordinator returned comments on 18 fusion research start-up reports, followed by discussion on research directions for the next fiscal year.

Start-up support for new appointments and fusion research: In FY2024, start-up support for new appointments (4.4 million yen for 4 new positions) and start-up support for fusion research to take on challenging bottom-up fusion projects (17 projects (17 million yen) and 1 group project (5 million yen) for a total of 22 million yen) were awarded.

Papers in collaborations: In 2024, the center has achieved outstanding research achievements. 188 papers including 21 TOP 10% papers (11% of 188 total papers, university average 9%), with more than 20 per year Top 10% papers from 2020 to 2024 (see table below) and 49 highly cited papers (IF 9 or more) were published in peer-reviewed journals which is 3 times (9 papers per PI and Jr-PI) the number of papers published by professors of the University per year (3 papers). 6 papers were in journals with IF > 20, and 33 papers were in journals with 20 > IF > 10. One paper was published in *Nature* (IF: 50.5), one in *Science* (IF: 44.8), and one in *Advanced Materials* (IF: 27.4), one in *Advance Energy Materials* (IF: 24.4), one in *Cell Host & Microbe* (IF: 20.6). Since the establishment of the center, the center has been actively collaborating with domestic and international researchers as well as promoting fusion research within the center, leading to collaborative papers within Hokkaido University (52), with domestic collaborators (63), and with international collaborators (72; 39% of papers from the center) in 2024.

Year	2018	2019	2020	2021	2022	2023	2024
Papers	5	89	133	180	143	180	188
Papers in Top10%	2	15	25	31	21	22	21
%Papers in Top10%	40%	17%	18%	17%	15%	12%	11%

Interdepartmental joint symposiums: The 10th Hokkaido University Cross-Departmental Symposium was held on September 6th, 2024, which aims to promote exchange among young researchers within Hokkaido University and the creation of fusion research. This symposium had 825 participants. Professor Hiroshi Amano (Nagoya University, Nobel Laureate in Physics 2014) made a special lecture, 3 center-related faculty members presented two oral and one poster presentations. Two center-related faculty members received awards at the symposium, including the 2024 Hokkaido University Research Encouragement Award (1 faculty members), Best Presentation Award (1 faculty members).

Pre-checking system for the grant application: The center conducted a pre-checking system to review and revise the applications for Grants-in-Aid for Scientific Research, etc. before submission. 48% of the applications for Grants-in-Aid for Scientific Research, including "Transformative Research Areas A", were granted for FY2024 (see below). The amounts of Grants-in-Aid for Scientific Research obtained have been increasing every year. FY 2018: 78 million yen, FY 2019: 159 million yen, FY 2020: 148 million yen, FY 2021: 182 million yen, FY2022: 219 million yen, FY2023: 288 million yen, FY2024: 333 million yen and overseas PIs, Jr-PIs, and young researchers have also succeeded in obtaining Grants-in-Aid for Scientific Research.

Scientific Research A	Scientific Research B	Scientific Research C	Scientific Research on Innovative Areas	Challenging Research (Exploratory)	Transformative Research Areas A	Transformative Research Areas B	Early-Career Scientists	Total	Average of adoptions for the center	Average of adoptions for the university

FY2025 number of adoptions / applications	0/0	2/6	3/5	0/0	0/0	2/7	0/0	6/9	13/27	48.1%	36.3%
FY2024 number of adoptions / applications	0/0	0/3	1/5	0/0		3/9	0/1	5/7	9/25	36.0%	34.7%
FY2023 number of adoptions / applications	0/0	0/4	0/4	0/0		0/0	4/4	7/15	11/27	40.7%	38.3%
FY2022 number of adoptions / applications	0/0	1/4	1/4	0/0		1/3	0/3	4/9	7/23	30.4%	37.1%
FY2021 number of adoptions / applications	0/1	2/6	3/5	1/1		-	-	6/14	12/27	44.4%	38.0%
FY2020 number of adoptions / applications	0/1	1/3	0/1	1/3		-	-	3/7	5/15	33.3%	37.1%

Securing research funding: The center's PIs and other researchers have continued to receive competitive research funding steadily since its inception. The total amount of these funds was 203 million yen in 2018, 668 million yen in 2019, 934 million yen in 2020, 655 million yen in 2021, 843 million yen in FY2022, 1,273 million yen in FY2023, and 1,212 million yen in FY2024. Representative competitive research funds in FY2024 are Grants-in-Aid for Scientific Research "Fund for the Promotion of Joint International Research (International Leading Research)" (1) and "Scientific Research S" (2), JST-ERATO (1), JST-CREST (3), JST-FOREST (6), JST-PRESTO (2), AMED-PROMOTE (2), AMED-SENTAN (1) etc.

3. Realizing an International Research Environment

* Describe what's been accomplished in the efforts to raise the center's recognition as a genuine globally visible research institute, along with innovative efforts proactively being taken in accordance with the development stage of the center, including the following points, for example:

- Efforts being developed based on the analysis of number and state of world-leading, frontline researchers (in Appendix 2); exchanges with overseas entities (in Appendix 4); number and state of visiting researchers (in Appendix 5)
- Proactive efforts to raise the level of the center's international recognition
- Efforts to make the center into one that attracts excellent young researchers from around the world (such as efforts fostering young researchers and contributing to advancing their career paths)

- (1) **Number of researchers:** The center conducted an international call for applications for new specially appointed faculty members and postdoctoral researchers to be hired at the center and received many applications from home and abroad in FY2024 (122 applications for 15 positions). As of March 31, 2025, the number of PIs was 15, including 3 foreign PIs, 41% of all researchers were foreign nationals, and 16% were female researchers (a total of 79 researchers, including 32 foreign nationals and 13 female researchers, divided into the fields of computation (16 researchers, 20%), information (20 researchers, 25%), and experiment (43 researchers, 55%)). The ratio of research fields is about 4:6 for computation/information to experimental Science, which sufficiently covers all research fields to strengthen the mission of the center. Furthermore, temporary childcare spaces were set up in the CRIS Building and ICRReDD building in FY2023, providing a space that ICRReDD researchers can use to care for their children.
- (2) **ICRReDD International symposium:** Since 2021, the center established the Akira Suzuki and ICRReDD Awards, which honor prominent chemists in both experimental chemistry and computational chemistry or information science. The 4th annual awards were given to Professor Gregory C. Fu of the California Institute of Technology and Professor Alán Aspuru-Guzik of the University of Toronto, strengthening the center's connection with these two prominent scientists and their institutions. Each fiscal year, the center has held the ICRReDD international symposium, inviting researchers from Japan and overseas to introduce them to the vision and research of the center. The 8th ICRReDD international symposium and the 2nd "Rising Star Program" by Junior PIs were jointly held on October 22nd and 24th, 2024. The symposium had 642 total participants (398 on-site and 244 online), Total of 54 participants from overseas (15 countries), and 52 poster sessions. Speakers of 8th symposium were Gregory C. Fu (Caltech, Akira Suzuki Award winner), Alán Aspuru-Guzik (Univ. of Toronto, ICRReDD Award winner), Panče Naumov (New York Univ. Abu Dhabi), Leroy Cronin (Univ. of Glasgow), Mary P. Watson (Univ. of Delaware), Corinna Schindler (Univ. of British Columbia), Varinder K. Aggarwal (Univ. of Bristol), Aiichiro Nagaki (Hokkaido Univ.), Hideyuki Otsuka (Science Tokyo) and ICRReDD's Ichigaku Takigawa, Toshifumi Satoh and Keisuke Takahashi. Speakers of Rising Star Program were Donald A. Watson (Univ. of Delaware), Derek Ahneman (IBM Research), Miho Hatanaka (Keio

Univ.), Ryo Tamura (NIMS), David A. Nagib (Ohio State Univ.), Jeehyun Yang (NASA Jet Propulsion Lab.) and ICRéDD's Tasuku Nakajima. The 2nd "List Sustainable DX Catalyst Collaboration Platform (List-PF)" Symposium was held on August 29th, where Professors List, Shimizu, Takahashi and Jin (Junior PI) from ICRéDD and two invited speakers, Professors Yamamoto (Chubu Univ.) and Harada (Chiba Univ.), gave lectures. The symposium had 78 participants, including five distinguished leading researchers in the field of organocatalytic chemistry (Platform Fellows). Hiroshima University WPI-SKCM² and ICRéDD held a joint international symposium on July 11. Both WPI centers presented their latest research and 114 people (86 in person and 28 online) attended the symposium. Speakers of SKCM² were Katsuya Inoue, Danny Hsu, Hiroshi Sato and ICRéDD's Yasuchika Hasegawa, Jian Ping Gong and Hajime Ito.

- (3) **International seminars:** In FY2024, the center held 16 international seminars. Speakers for the seminars were Christina W. Li (Purdue Univ., May 9), Christopher H. Uyeda (Purdue Univ. May 10), Vladimír Malkin and Olga L. Malkina (Slovak Academy of Sciences, Jun. 26), Djamaladdin G. Musaev (Emory University, Jul. 16), Byeong-Su Kim (Yonsei Univ., Jul. 22), Odile Eisenstein (Univ. Montpellier, Aug. 21), Hao Guo (Duke Univ., Sept. 3), Seung Hwan Cho (POSTECH, Oct. 4), Rui Shang (Univ. of Tokyo, Oct. 17), David Wales (Univ. of Cambridge, Nov. 21), Malcolm D. E. Forbes (Bowling Green State Univ., Dec. 3), C. Malla Reddy (Indian Inst. of Tech., Dec. 12), Tokushi Sato (EuXFEL, Jan. 8), Magdalena Skipper (Editor in Chief, Nature, Feb. 10), Vincent Robert (Univ. de Strasbourg, Mar. 12). Such seminars will be held regularly in the future.
- (4) **Other seminars and symposia:** Several seminars and symposia were held to ensure opportunities for regular and active communication in a cross-disciplinary manner among the center's young researchers, to advance future fusion research, and to solicit and propose new collaborative research. These events include five co-organized symposiums: SMCR (Soft Matter Collaborative Research Unit) Seminar 2024 by Prof. Michael Rubinstein (Aug. 26 and 28), 10th HU Cross-Departmental Symposium (Sep. 6), The 62nd Aurora Seminar by the Catalysis Society Japan (Oct. 25), ISAJ (Indian Scientist Association in Japan) Symposium (Dec. 13), LeNet (JSPS international leading research project "Design of Low Entropy Polymer Network Materials for Unique Functions", which is a collaborative project between Japan, U.S., and EU teams, focuses on low entropy polymer networks (LeNet) that realize unique mechanical properties and functions derived from their low-entropy structures) International Symposium (Feb. 12-14), and two research ethics seminars (Satoshi Iimuro (Nov. 12) and Iekuni Ichikawa (Nov. 13).
- (5) **Fostering young researchers by MANABIYA:** Researchers were accepted through the MANABIYA system. "MANABIYA (ACADEMIC)" invited applications from March 2024 and accepted 24 researchers (7 were accepted from within Japan and 17 were accepted from abroad) out of 29 applicants, who were trained in the center's techniques.

4. Making Organizational Reforms

- * Describe the system reforms made to the center's research operation and administrative organization, along with their background and results.
- * Describe the measures you've taken and results achieved in implementing the center's gender-balance plan. Describe also your measures/results for fostering researchers with a view to achieving your gender plans and for conducting domestic and international promotion activities to attract female researchers to the center.
- * If innovated system reforms generated by the center have had a ripple effect on other departments of the host institutions or on other research institutions, clearly describe in what ways.
- * Describe the center's operation and the host institution's commitment to the system reforms. (Include measures taken by the host institution to provide a support system and to work toward improving the environment for achieving gender balance.)

- (1) **Evaluation system of center faculty members:** In FY2022, a new regulation was established to provide incentives based on the research performance and discretionary evaluation by annual interview of center faculty members, for whom no evaluation system was previously in place. The results of the self-performance evaluation, and discretionary performance evaluation based on annual interview with the Center Director are used to determine the salary increase or decrease by one or two steps from the base annual salary for the following year, which has not yet been done in any other departments in the University. Performance evaluations (S, A, B, C and D) were conducted for 13 faculty members, excluding those who arrived and left during FY2024. 3 faculty members received a two-level salary increase for evaluation grade S, 6 faculty members received a one-level salary increase for evaluation grade A, 2 faculty members received no revision salary for evaluation grade B, 2

faculty members received a one-level salary decrease for evaluation grade C and no faculty member received a two-level salary decrease for evaluation grade D. In FY2025, a new provision was established to provide postdoctoral fellows, for whom there had been no incentive system, to receive rewards for research papers with >10 IF.

- (2) **Establishment of ICReDD fellow system**: Since FY2023, the center established a new position called the ICReDD fellow to expand ICReDD's research activities inside and outside the university and to serve as an incubation system for new PIs. In FY2024, two professors were appointed. The center provides ICReDD fellows with our resources and we collaborate with them. When a senior PI is to be replaced or new developments in research are needed, the most suitable ICReDD fellow is selected. The center will be made a permanent research center that always promotes cutting-edge, world-class research based on a new adaptive research strategy involving periodically changing researchers and research themes.
- (3) **The decision-making system**: The mission of the center is communicated to all members through interviews with researchers at the time of hire and annually by the Center Director. In the case of mixed laboratories and offices, a laboratory chief is appointed to manage the laboratories and ensure that the Center Director's policies are promptly communicated. Under the direct control of the Center Director, a Fusion Research Coordinator, who is directly connected to the research division, has been established in FY2022 to actively promote, plan, and advise on the progress of fusion research. In addition, the authority was delegated to the Future Planning Working Group and the Equipment Management Working Group so that they can manage the center under the direction of the Center Director. The Advisory Board Meeting, which meets regularly, was established to obtain advice, recommendations, and evaluations from experts on future perspectives, strategies, and approaches to problem-solving approaches to realize the center's vision and form a world-class research center, and to contribute to the future operation of the center. The Advisory Board online meetings were held on March 13 (European members) and 21 (U.S. and Canadian members). Board members reviewed progress and follow-up reports from an international perspective, made recommendations on the future direction of the center, and provided advice on how to promote research. In particular, the members suggested that (i) it is important to secure a budget to make the center permanent in the future, (ii) the Data Management Team and the DEI Promotion Team have been established and should be continued, and (iii) to improve the gender balance, it is important to actively invite female researchers as speakers for symposia and seminars, and to continuously show career paths to students and young researchers.
- (4) **Strengthen the research support system**: Under the direction of the Administrative Director, the General Affairs Unit, International Planning Unit, Research Strategy Unit, and Human Resources Development Unit functionally collaborated to manage the center. In FY2024, the DEI Promotion Team was established to develop measures to improve the gender balance of the center. The action plans were (i) to accelerate the increase of the proportion of female professors (ICReDD fellows or collaborators), (ii) to promote a limited open application for female faculty members and postdoctoral fellows, and (iii) to organize events for the project to support female junior and senior high school students in choosing careers in chemistry or information science in cooperation with the university office of the DEI. In addition, the "Fusion Research Coordinator" and the "Data Management Team" have been directly attached to the Research Division, to manage the Center Director's policies and monitor progress in close coordination with researchers.
- (5) **The center's gender-balance plan: The center will take various measures to ensure the diversity of its members, especially to achieve an appropriate gender balance.** Achieving an appropriate gender balance at the center is one of our top priorities and the center aims to achieve a gender balance of 25% (18% as of March 2025). In FY2025, the center has increased the number of female PIs from two to three and will increase the number of female Jr-PIs from one to two. The total goal of 25% female researchers is broken down into specific goals for different seniority levels, with a goal of 20% females at the executive level (Center Director, Administrative Director, etc), 13% at the principal investigator level (professors and associate professors) and 27% among other researchers. To achieve this goal, all PI-groups are asked to have at least one female researcher. The university already secured positions for a female assistant professor and a tenure-track associate professor for the center. In the future, the center plans to recruit several open positions for female-only faculty members. Through these positions, a career path system for female researchers from student, postdoctoral

researcher, assistant professor, and associate professor (Jr. PI) to professor (PI), can be expected to function as a role model for and attract more attention from female researchers. Finally, they will be established as PIs of the center and inject a fresh, young perspective into the center's research direction and leadership. The center periodically conducts seminars and other events that contribute to the promotion of diversity, equity, inclusion, and gender balance for members of faculty, staff, students, etc. The center will also actively recruit female faculty members and students using the University Accelerated Gender Balance Action Plan and the University Fellowship System, and establish a strong, collaborative relationship with the Office of Diversity, Equity, and Inclusion.

5. Efforts to Secure the Center's Future Development over the Mid- to Long-term

* Address the following items, which are essential to mid- to long-term center development:

- Future prospects with regard to the research plan, research organization and PI composition; prospects for achieving gender balance; prospects for fostering and securing of next-generation researchers.
- Prospects for securing resources such as permanent positions and revenues; plan and/or implementation for defining the center's role and/or positioning the center within the host institution's institutional structure
- Measures to sustain the center as a world premier international research center after program funding ends
- Host institution's organizational reforms carried out for the center's autonomous administration simultaneously with the creation of the center.

The university highly evaluates the center's achievements and plans to expand these achievements to other departments of the university, such as a management system that clearly separates research and administrative organization, like a Center Director and Administrative Director, a careful performance evaluation system that provides incentives to faculty members and postdoctoral fellows, a hospitality system that supports the daily life of foreign researchers, DEI Promotion Team that develops measures to improve the gender balance of the center and the assignment of faculty members specializing in fusion research (Fusion Research Coordinator) and an instrument management faculty member to prevent research misconduct.

- (1) **Financial support:** Since the establishment of the center, Hokkaido University has strongly supported the center and has secured funds equal to or more than the WPI grant for its operation (FY2018: 358 million yen, FY2019: 1,026 million yen, FY2020: 1,388 million yen, FY2021: 1,904 million yen, FY2022: 2,620 million yen, FY2023: 1,830 million yen, FY2024: 1,685 million yen). The university also provides the center with full access to its financial infrastructure, i.e., the opportunity to request budget estimates and to apply for competitive cross-departmental funding. In FY2024, The List-DX Catalyst Collaboration Research Platform (List-Platform) which was launched in FY2023 for the further development of research and enhancement of domestic and international research hub functions, held international symposium on August, initiated 9 joint research projects with companies and 33 papers on research results (including 13 international co-authored papers) were published to promote the platform's research. Since June 2021, GRRM20 was launched by HPC Systems, Inc. under a program license agreement with the University, and license income has been increasing year by year. The five-year large-scale joint research project (totaling 250 million yen) with Mitsui Chemicals, which was launched in FY2023, made successful progress, including the acquisition of patents, etc. MANABIYA (INDUSTRY) was contracted for 16 projects (4 consultants and 12 joint research projects) to expand the network with companies in related fields. In FY2023, a start-up (MECHANOCROSS Co., Ltd.) associated with Flagship Project IV was launched. In this way, from FY2025, the center will gradually secure continuous research funding and become independent by decreasing the proportion of the university's voluntary cost burden.
- (2) **Personnel support:** To ensure that the center sustainably continues its research activities independently, the university provided financial support for tenure-track positions that were offered to outstanding WPI researchers. These were appointed following a rigorous selection process based on research activities such as high-impact publications and receipt of competitive funds. The university also decided to secure one associate professor as a Junior PI for the center in FY2025. In the future, one regular associate professor and one post-doctoral researcher will be assigned to each senior PI of the center and the six Junior PIs will be assigned one post-doctoral fellow each. Starting in FY2024, the university has decided to gradually secure personnel expenses to the center equivalent to 13 professors.
- (3) **Support system and environmental improvement for achieving gender balance:** The university developed a policy for improving gender balance (Ratio of female faculty members:

23% by 2028) based on the university's program "Accelerate Ambitious of All", adopted as part of the MEXT subsidy program "The Initiative for Realizing Diversity in the Research Environment (leadership training for women)" (FY2023-FY2028). Aiming to accelerate the increase of the ratio of women in upper-level and managerial positions, the University has established the "Support for Female Students and Graduate Students Entering Doctoral Programs," "Support for Invitation of Female Researchers," "Support for the Employment of Technical Assistants over Life Events," "Mentoring & Job Shadowing Training Support Program for Female Researchers Pursuing Higher Positions," and "Support for Female Researchers to be Hired and to be Proactively Assigned to Upper-Level Positions." The university established the "Accelerated Action Plan to Promote Recruitment and Active Promotion of Female Researchers to Higher Positions" to promote 25 female associate professors to professorships in FY2023. 34 applications were received, and a total of 25 professors (17 in Natural Sciences and 8 in Humanities and Social Sciences) were promoted. As a result, the percentage of female professors increased from 7.4% to 10.4%. The university set a target of 20% female professors by FY2028. At ICReDD, one female researcher took advantage of "Support for the Employment of Technical Assistants over Life Events" and a research assistant staff was hired during her childcare leave (FY2021), which led to a smooth return to research activities after she returned to work. The university also established the "Yoshie Katsurada Award," named after Hokkaido University's first female professor, to honor female faculty members who have developed outstanding academic research and are expected to be active in the next generation of management positions, and in FY2023, four female researchers, including one PI, received this award, and in FY2024, four female researchers received this award.

- (4) **Technical support:** The university established an integrated technical staff organization, the Office for Technical Support, to which technical staff members from various departments in the university were dually appointed, and the consolidation of the centralized administrative system within its operating structure strengthens the support system for cross-divisional education and research activities. In response to a request from the center, the Office for Technical Support dispatched technical staff, performing duties in cooperation with the equipment management faculty members to assist in the maintenance and management of the center's equipment (nuclear magnetic resonance equipment) under the coordination with the Equipment Management Working Group. The university provided the fees required to analyze synthesized samples in research projects of the center, as well as the usage fees for the open facility system, which provides access to cutting-edge equipment such as high-resolution NMR spectrometers that are managed by the university (FY2019: 850,000 yen; FY2020: 1 million yen; FY2021: 2.5 million yen; FY2022: 2.3 million yen, FY2023: 4.3 million yen, FY2024: 4.7 million yen).
- (5) **Establishment of graduate school:** In FY2024, the Laboratory of Chemical Reaction Design and Discovery, consisting of 7 professors and 7 graduate students, was established in the Graduate School of Chemical Sciences and Engineering. To incorporate the world's most advanced research back into educational programs, the university plans to establish a system for cross-disciplinary and interdisciplinary education that is not bound by the framework of existing research institutes and graduate schools. The center established the "Human Resource Development Unit" to design a human resource development framework that served as a model case for next-generation higher education through a multilateral approach for students and working people regardless of national or international affiliation. In FY2024, full-time and specialized faculty members of the Human Resource Development Unit developed a curriculum and began preparations to establish an ICReDD course in the Graduate School of Chemical Sciences and Engineering starting in FY2028. Furthermore, the educational reform of a research institution having its own graduate school is worthy of attention not only for its impact within the university but also outside the university, and as an attempt to foster human resources to take responsibility for the world-leading-edge research.

6. Others

* Describe what was accomplished in the center's outreach activities last year and how the activities have contributed to enhancing the center's "globally visibility." In Appendix 6, describe concretely the contents of these outreach activities. In Appendix 7, describe media reports or coverage, if any, of the activities.

* In addition to the above 1-5 viewpoints, if there is anything else that deserves mention regarding the center project's progress, note it.

- (1) In FY2024, the ICRéDD International Symposium and the "Rising Star Program", which are originally two independent events, were jointly held as a large three-day symposium. ICRéDD invited a wide range of presenters from Japan and abroad, with the privilege of supporting travel expenses for the best students among the poster presentation applicants. The total number of presenters was 52 (39 students and 13 researchers), of which 2 students from Japan and 1 student from Thailand were supported with travel expenses. The breakdown of the 52 presenters' affiliations is: 36 from Hokkaido University, 8 from other domestic institutions, and 8 from four foreign institutions. The total number of presenters increased by 2.4 times (57% increase) and the total number of participating countries increased from 3 to 5, as 22 (19 from Hokkaido University, 1 from another domestic institution, and 2 from 2 foreign countries) presented posters in the previous year's Rising Star Program.
- (2) The center has world-class researchers as Principal Investigators (PIs) and has received outstanding awards such as 2024 Royal Society of Chemistry Horizon Prize (NSF Center for molecularly Optimized Networks (Gong, Rubinstein and 17 researchers). In FY2024, the center members have presented their research in 68 invited lectures at international conferences and received 17 awards.
- (3) The MANABIYA page on the ICRéDD website was reorganized and enhanced. In addition, a new pamphlet summarizing the MANABIYA application process was published and distributed at events and to visitors. As a result, 50 applications were received for the 2025 MANABIYA program, which was solicited in FY2024, a 1.7-fold increase (42% increase) over the 29 applications received in the previous year.
- (4) The center has published a "Monthly Research News Postcard" that provides monthly research highlights, a "Quarterly News Poster" that presents research content in an easy-to-understand manner, and an "Annual Report" to provide information on the center's annual research activities. Information was widely disseminated domestically and internationally. Our monthly research news postcard series promote our latest research to a mailing list of hundreds of people, including over 70 international addresses. A unique endeavor at the center is our quarterly news poster "The CATALYST", which explains chemical concepts of chemistry in an easy-to-understand manner, while also introducing the center's research to a high school-level, non-scientist audience via a 220-person mailing list. In FY2024, 3 issues were published in poster format: "Environmentally friendly reaction development; Force is the key? (Vol. 16)", "Designing crystals that spin (Vol. 17)", and "What is a reaction in the first place? (Vol. 18)". In addition, starting with the March 2025 issue, the magazine has been redesigned as "The Catalyst Newspaper" to focus on more familiar science topics in a newspaper style, with more pages and a larger circulation so that it can be read by more college and high school students.
- (5) Continuing from the previous year, Associate Professor Yu Harabuchi's project was selected for "Academic Fantasia," a research support program conducted by Hokkaido University in cooperation with the Hokkaido Shimbun to promote "science and technology dialogue with the public," and through this program he gave classes and facility tours to two high schools in Hokkaido. One of the schools requested to participate in the next year's program, and we plan to continue this activity.

7. Center's Response to Results of Last Year's Follow-up

* Transcribe the item from the "Actions required and recommendations" section in the site visit report and the Follow-up report, then note how the center has responded to them.

* If you have already provided this information, indicate where in the report.

- 1) Continue the effort to achieve top-level science through fusion of computation / informatics / experiment. Flagship projects are full of seeds for achieving pioneering breakthroughs in chemical reaction design and discovery.

In flagship project 1, theoretical methods, database construction has progressed and AI-based analysis techniques have been developed. In flagship project 2, quantum chemistry-based ab initio reaction design has progressed, enabling retrosynthesis approaches and strategic reaction design. In flagship project 3, catalyst design, new AI-driven catalyst design has progressed, supported by automated synthesizers. In flagship project 4, mechanochemical synthesis, several new reactivities in ball-mill synthesis were discovered, and the theory of reaction kinetics in response to rheology-based mechanical stimuli was deepened. In the polymer field of flagship

project 5, a new methodology for polymer synthesis has been established, and new chemical reactions utilizing radical reactions are being realized. The application of cancer stem cells to the biological field of flagship project 6 has progressed and research combined with information technology has also progressed.

2) Continue the effort to improve gender balance at all levels, particularly at the PI level.

The center's philosophy is to reflect and activate the improvement of gender balance and diversity inclusion in the center's research and operations. The future vision of the center aims to achieve a gender balance of 25% (18% as of March 2025). In FY2025, the center increased the number of female PIs from two to three and will increase the number of female Jr-PIs from one to two. The action plans developed by the DEI Promotion Team were (i) to accelerate the increase of the proportion of female professors (ICReDD fellows or collaborators), (ii) to promote a limited open application for female faculty members and postdoctoral fellows, and (iii) to organize events for the project to support female junior and senior high school students in choosing careers in chemistry or information science in cooperation with the university office of the DEI. The center will improve the gender balance by actively inviting female researchers as lecturers at symposia and seminars, and by continuously presenting career paths to students and young researchers. At the 9th ICReDD International Symposium in October 2025, 58% of all speakers will be female researchers.

3) Speed up the planning of the ICReDD (MANABIYA)-based new graduate school.

In FY2024, the Laboratory of Chemical Reaction Design and Discovery, consisting of 7 professors and 7 graduate students, was established in the Graduate School of Chemical Sciences and Engineering. In FY2025, the number of professors and graduate students will be 10 and 10, respectively. In addition, master's students who wish to advance the Ph.D. program in the ICReDD laboratory will be hired as RAs. In FY2024, full-time and specialized faculty members of the Human Resource Development Unit developed a curriculum and began preparations to establish an ICReDD course in the Graduate School of Chemical Sciences and Engineering starting in FY2028.

4) International interactions of junior researchers from ICReDD are an area to improve. It is recommended that supporting systems be established to encourage ICReDD's young PIs, young scientists and even graduate students to take advantage of opportunities for international exposure to enhance their value early in their scientific careers.

Since FY2024, the center has established a system for inviting prominent overseas researchers with the aim of strengthening the international presence of the center by promoting the formation and internationalization of the center through the organization of meetings and seminars for the promotion of flagship projects. Six overseas researchers have been invited to the center. The center established some supporting systems to encourage ICReDD's young PIs, young scientists, and even graduate students to take advantage of opportunities for international exposure to enhance their value early in their scientific careers. In FY2023, the ICReDD Rising Star Program was launched to provide Jr-PIs and young researchers with more opportunities to communicate with the world's top researchers by entrusting them with symposium planning/management. In FY2024, the ICReDD International Symposium and the "Rising Star Program", which are originally two independent events, were jointly held as a large three-day symposium. ICReDD invited a wide range of presenters from Japan and abroad, with the privilege of supporting travel expenses for the best students among the poster presentation applicants. In FY2025, the center also has established a new ICReDD Lectureship Support/Award, which support travel expenses for research exchange activities conducted at overseas research institutions within 2 weeks, to encourage early-career researchers to actively engage with international research communities and build collaborative research frameworks with leading research groups abroad.

Appendix 1 FY 2024 List of Center's Research Results and Main Awards

1. Refereed Papers

- List only the Center's papers published in 2024. (Note: The list should be for the calendar year, not the fiscal year.)

- (1) Divide the papers into two categories, A and B.
 - A. WPI papers
List papers whose author(s) can be identified as affiliated with the WPI program (e.g., that state "WPI" and the name of the WPI center (WPI-center name)). (Not including papers in which the names of persons affiliated with the WPI program are contained only in acknowledgements.)
 - B. WPI-related papers
List papers related to the WPI program but whose authors are not noted in the institutional affiliations as WPI affiliated. (Including papers whose acknowledgements contain the names of researchers affiliated with the WPI program.)

Note: On 14 December 2011, the Basic Research Promotion Division (the Basic and Generic Research Division at present) in MEXT's Research Promotion Bureau circulated an instruction requiring paper authors to include the name or abbreviation of their WPI center among their institutional affiliations. From 2012, the authors' affiliations must be clearly noted.

- (2) Method of listing paper
 - List only refereed papers. Divide them into categories (e.g., original articles, reviews, proceedings).
 - For each, write the author name(s); year of publication; journal name, volume, page(s) (or DOI number), and article title. Any listing order may be used as long as format is consistent. (The names of the center researchers do not need to be underlined.)
 - If a paper has many authors (say, more than 10), all of their names do not need to be listed.
 - Assign a serial number to each paper to be used to identify it throughout the report.
 - If the papers are written in languages other than English, underline their serial numbers.
 - Order of Listing
 - A. WPI papers
 1. Original articles
 2. Review articles
 3. Proceedings
 4. Other English articles
 - B. WPI-related papers
 1. Original articles
 2. Review articles
 3. Proceedings
 4. Other English articles
- (3) Submission of electronic data
 - In addition to the above, provide a .csv file output from the Web of Science (e.g.) or other database giving the paper's raw data including Document ID. (Note: the Document ID is assigned by paper database.)
 - The papers should be divided into A or B categories on separate sheets, not divided by paper categories.
- (4) Use in assessments
 - The lists of papers will be used in assessing the state of WPI project's progress.
 - They will be used as reference in analyzing the trends and whole states of research in the said WPI center, not to evaluate individual researcher performance.
 - The special characteristics of each research domain will be considered when conducting assessments.
- (5) Additional documents
 - After all documents, including these paper listings, showing the state of research progress have been submitted, additional documents may be requested.

A. WPI papers

1. Original articles

- (1) Abedin, M.; Tabata, K.; Matsumura, Y.; Komatsuzaki, T. Multi-armed bandit algorithm for sequential experiments of molecular properties with dynamic feature selection. *JOURNAL OF CHEMICAL PHYSICS* **2024**, *161* (1). DOI: 10.1063/5.0206042.
- (2) Akhmetshin, T.; Zankov, D.; Gantzer, P.; Babadeev, D.; Pinigina, A.; Madzhidov, T.; Varnek, A. SynPlanner: An End-to-End Tool for Synthesis Planning. *JOURNAL OF CHEMICAL INFORMATION AND MODELING* **2024**, *65* (1), 15-21. DOI: 10.1021/acs.jcim.4c02004.
- (3) Amano, R.; Nishizawa, D.; Taketsugu, T.; Iwasa, T. Optical force and torque in near-field excitation of C₃H₆: A first-principles study using RT-TDDFT. *JOURNAL OF CHEMICAL PHYSICS* **2024**, *161* (12). DOI: 10.1063/5.0223371.

- (4) Andersson, R.; Johansson, I.; Shivakumar, K.; Hern, G.; Inokuma, Y.; Mindemark, J. Implementation of highly crystalline polyketones as solid polymer electrolytes in high-temperature lithium metal batteries. *SOLID STATE IONICS* **2024**, *410*. DOI: 10.1016/j.ssi.2024.116542.
- (5) Begum, M.; Lama, M.; Yang, W.; Li, X.; Haque, M.; Li, X.; Gong, J. Fatigue Behaviors of Anisotropic Hydrogels with a Macroscopic Lamellar Bilayer Structure and Swelling Effects. *MACROMOLECULES* **2024**. DOI: 10.1021/acs.macromol.4c01698.
- (6) Blancas, E.; Lobato, A.; Izquierdo-Ruiz, F.; Márquez, A.; Recio, J.; Nath, P.; Plata, J.; Otero-de-la-Roza, A. Thermodynamics of solids including anharmonicity through quasiparticle theory. *NPJ COMPUTATIONAL MATERIALS* **2024**, *10* (1). DOI: 10.1038/s41524-024-01447-8.
- (7) Blum, V.; Asahi, R.; Autschbach, J.; Bannwarth, C.; Bihlmayer, G.; Blügel, S.; Burns, L.; Crawford, T.; Dawson, W.; de Jong, W.; et al. Roadmap on methods and software for electronic structure based simulations in chemistry and materials. *ELECTRONIC STRUCTURE* **2024**, *6* (4). DOI: 10.1088/2516-1075/ad48ec.
- (8) Chan, B.; Rubinstein, M. Activity-driven chromatin organization during interphase: Compaction, segregation, and entanglement suppression. *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA* **2024**, *121* (21). DOI: 10.1073/pnas.2401494121.
- (9) Chen, K.; Lee, C.; Chen, C.; Satoh, T.; Isono, T.; Chen, H. Phase Behavior of Sugar-based Block Copolymer Modulated by Molecular Chirality. *GIANT* **2024**, *19*. DOI: 10.1016/j.giant.2024.100308.
- (10) Debbarma, S.; Hayashi, H.; Ueno, Y.; Kanna, W.; Tanaka, K. I.; Mita, T. Photoredox-Catalyst-Free Carboxylation of Unactivated Alkenes in DMSO: Synthesis of Polycyclic Indole Derivatives and Aliphatic Acids. *ORGANIC LETTERS* **2024**, *26* (50), 10897-10902. DOI: 10.1021/acs.orglett.4c04051.
- (11) Dostagir, N.; Tomuschat, C.; Oshiro, K.; Gao, M.; Hasegawa, J.; Fukuoka, A.; Shrotri, A. Mitigating the Poisoning Effect of Formate during CO₂ Hydrogenation to Methanol over Co-Containing Dual-Atom Oxide Catalysts. *JACS AU* **2024**, *4* (3), 1048-1058. DOI: 10.1021/jacsau.3c00789.
- (12) Ducloué, L.; Haque, M.; Goral, M.; Ilyas, M.; Gong, J.; Lindner, A. Color-switching hydrogels as integrated microfluidic pressure sensors. *SCIENTIFIC REPORTS* **2024**, *14* (1). DOI: 10.1038/s41598-024-56140-z.
- (13) Fan, H.; Naohara, D.; Li, W.; Li, X.; Gong, J. Tuning network structures of hydrophobic hydrogels by controlling polymerization solvent. *POLYMER CHEMISTRY* **2024**, *15* (20), 2104-2111. DOI: 10.1039/d4py00256c.
- (14) Fujii, S.; Yaguchi, H.; Takahashi-Iwata, I.; Inoue, T.; Tarisawa, M.; Nomura, T.; Kudo, A.; Uwatoko, H.; Shirai, S.; Matsushima, M.; et al. Anti-Tr/DNER Antibody-associated Paraneoplastic Neurological Syndrome Presenting Limbic Encephalitis with Anaplastic Large Cell Lymphoma: A Case Report. *INTERNAL MEDICINE* **2024**. DOI: 10.2169/internalmedicine.4530-24.
- (15) Fujita, H.; Arai, S.; Arakawa, H.; Hamamoto, K.; Kato, T.; Arai, T.; Nitta, N.; Hotta, K.; Hosokawa, N.; Ohbayashi, T.; et al. Drug-drug conjugates of MEK and Akt inhibitors for RAS-mutant cancers. *BIOORGANIC & MEDICINAL CHEMISTRY* **2024**, *102*. DOI: 10.1016/j.bmc.2024.117674.
- (16) Fujita, S.; Plianchaisuk, A.; Deguchi, S.; Ito, H.; Nao, N.; Wang, L.; Nasser, H.; Tamura, T.; Kimura, I.; Kashima, Y.; et al. Virological characteristics of a SARS-CoV-2-related bat coronavirus, BANAL-20-236. *EBIOMEDICINE* **2024**, *104*. DOI: 10.1016/j.ebiom.2024.105181.
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- (18) Gantzer, P.; Staub, R.; Harabuchi, Y.; Maeda, S.; Varnek, A. Chemography-guided analysis of a reaction path network for ethylene hydrogenation with a model Wilkinson's catalyst. *MOLECULAR INFORMATICS* **2025**, *44* (1). DOI: 10.1002/minf.202400063.
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- (175) Matsumoto, H.; Iwai, T.; Sawamura, M.; Miura, Y. Continuous-Flow Catalysis Using Phosphine-Metal Complexes on Porous Polymers: Designing Ligands, Pores, and Reactors. *CHEMPLUSCHEM* **2024**, *89* (10). DOI: 10.1002/cplu.202400039.
- (176) Qi, Y.; Fan, H. Recent Progress on Water-based Liquid Embolic Agents in Endovascular Treatment. *CHEMICAL RESEARCH IN CHINESE UNIVERSITIES* **2024**, *40* (5), 776-785. DOI: 10.1007/s40242-024-4060-2.
- (177) Wang, M.; Kitagawa, Y.; Hasegawa, Y. Current Development of Lanthanide Complexes for Biomedical Applications. *CHEMISTRY-AN ASIAN JOURNAL* **2024**, *19* (7). DOI: 10.1002/asia.202400038.
- (178) Watanabe, K.; Pati, N.; Inokuma, Y. Contracted porphyrins and calixpyrroles: synthetic challenges and ring-contraction effects. *CHEMICAL SCIENCE* **2024**, *15* (19), 6994-7009. DOI: 10.1039/d4sc02028f.

3. Proceedings

- (179) Nie, Y.; Sun, Y.; Tsuda, M.; Wang, L.; Gong, J.; Tanaka, S. Investigation of cancer stem cell generation by simulating hydrogel-based tumor microenvironment. *CANCER SCIENCE* **2024**, *115*, 1352-1352.
- (180) Sun, Y.; Nie, Y.; Tsuda, M.; Wang, L.; Gong, J.; Tanaka, S. Analysis of the effect of stiffness of cancer microenvironment on stemness induction of cancer cells using hydrogels. *CANCER SCIENCE* **2024**, *115*, 993-993.
- (181) Suzuka, J.; Saeki, S.; Kumegawa, K.; Ueno, T.; Tsuda, M.; Tanaka, S.; Maruyama, R. Analysis of plasticity of breast cancer cells focusing on dedifferentiation by hydrogel. *CANCER SCIENCE* **2024**, *115*, 843-843.
- (182) Tanaka, S. Novel cancer stem cell exploration- Expectations from pathology to spatial transcriptomes. *CANCER SCIENCE* **2024**, *115*, 815-815.
- (183) Wang, L.; Aoki, Y.; Tsuda, M.; Oda, Y.; Tanaka, S. Hydrogel PCDME creates pancreatic cancer stem cells in OXPPOS metabolic state with TXNIP elevation. *CANCER SCIENCE* **2024**, *115*, 1360-1360.

4. Other English articles

- (184) Komatsuzaki, T. An attempt of Seibutsu-Butsuri in Kyoto IUPAB Congress 2024. *BIOPHYSICAL REVIEWS* **2024**, *16* (5), 509-510. DOI: 10.1007/s12551-024-01241-2.

- (185) Konishi, T.; Funayama, N.; Hotta, D.; Tanaka, S. Acute eosinophilic myocarditis mimicking inferior myocardial infarction presenting with delayed hypereosinophilia. *CARDIOLOGY JOURNAL* 2024, 31 (2), 361-362. DOI: 10.5603/cj.96133.

B. WPI-related papers

1. Original articles

- (186) Liu, G.; Gao, W.; Huang, Z.; Sun, B.; Tong, Y.; Huang, G.; Fu, Y. Hydrogen behavior in Ti surface nitridation: Hydrogen as an active component catalyzes the nitridation reaction. *SURFACES AND INTERFACES* **2025**, 56. DOI: 10.1016/j.surfin.2024.105512.
- (187) Sharmin, N.; Islam, M.J. Photofunctionalized Europium(III) complexes with circularly polarized luminescence. *Chemical Physics Impact* **2025**, 10, 100806. DOI: 10.1016/j.chphi.2024.100806.
- (188) Yasumura, S.; Kato, T.; Qian, Y.; Toyao, T.; Shimizu, K. Mechanistic Study on NH₃ Decomposition over Cu-Exchanged CHA Zeolites Using Automated Reaction Route Mapping Combined with Neural Network Potential and Density Functional Theory Calculations. *JOURNAL OF PHYSICAL CHEMISTRY C* **2024**, 128 (31), 12949-12959. DOI: 10.1021/acs.jpcc.4c01831.

2. Review articles

3. Proceedings

4. Other English articles

2. Invited Lectures, Plenary Addresses (etc.) at International Conferences and International Research Meetings

- List up to 10 main presentations during FY 2024 in order from most recent.
- For each, write the date(s), lecturer/presenter's name, presentation title, and conference name.

Date(s)	Lecturer/Presenter's name	Presentation title	Conference name
March 25, 2025	Michael Rubinstein	The Art of Network Design	Spring Meeting of the American Chemical Society, San Diego, CA, USA
November 1, 2024	Benjamin List	"Universal Organocatalysts for our World"	Hongkong Future Science Prize Symposium, Hong Kong Special Administrative Region
September 2, 2024	Toshifumi Satoh	One-Step Synthesis of Multiblock Copolymers Using Alkali Metal Carboxylate Catalyst	15th International Symposium on Ionic Polymerization (IP'24), Mainz, Germany
August 20, 2024	Alexandre Varnek	"From Geography to Chemography and Back"	ACS meeting, Denver, USA
August 20, 2024	Satoshi Maeda	"First Principle Reactivity Exploration Using Artificial Forces"	15th Asian International Seminar on Atomic and Molecular Physics (AISAMP15), Daejeon, Korea
August 1, 2024	Tetsuya Taketsugu	"New techniques for understanding chemical reactions: a reaction space projector and a natural reaction orbital"	The 27th International Annual Symposium on Computational Science and Engineering (ANSCSE27), Chulalongkorn University, Thailand (keynote)
August 1, 2024	Yasuchika Hasegawa	HARD AND SOFT LANTHANIDE COORDINATION POLYMERS AND AGGREGATES FOR PHOTO-FUNCTIONAL MATERIALS	45th International Conference on Coordination Chemistry (ICCC) 2024 Colorado State University Fort Collins, Colorado State, USA
July 29, 2024	Jian Ping Gong	"Mechanochemistry in Double Network Materials"	The 8th International Soft Matter Conference (ISMC2024) Duke Soft Matter Day, Raleigh, North Carolina, USA
July, 15, 2024	Hajime Ito	Revolutionary Synthesis of Organometallic Compounds by Mechanochemical Method	30th International Conference on Organometallic Chemistry, Agra, India
June 25, 2024	Yasuhide Inokuma	Synthesis and properties of calix[3]pyrrole related macrocycles	The 13th International Conference on Porphyrins and Phthalocyanines (ICPP-13), Niagara Falls, Buffalo, USA

3. Major Awards

- List up to 10 main awards received during FY 2024 in order from the most recent.
- For each, write the date issued, the recipient's name, and the name of award.
- In case of multiple recipients, underline those affiliated with the center.

Date	Recipient's name	Name of award
January 6, 2025	Koji Kubota	Lectureship Award MBLA 2024, "Pioneering Solid-State Organic Synthetic Chemistry Using Mechanochemical Methods".
December 24, 2024	Hajime Ito	The Chemical Society of Japan Award for 2024, "Driving Innovations in Organic Synthesis and Organometallic Chemistry Based on Exploration of Solution and Solid-State Reactions"
December 24, 2024	Tsuyoshi Mita	The Chemical Society of Japan for Creative Work for 2024, "Development of Small-Molecule Activation Reactions and Reaction Design Using Quantum Chemical Calculations"
September 16, 2024	Tetsuya Taketsugu	The 15th Award of the Japan Society for Molecular Science, "Deepening the Understanding of Chemical Reaction Dynamics Based on the Concept of Reaction Pathways"
August 27, 2024	Michael Rubinstein	ACS Award in Polymer Chemistry, "his outstanding contributions for leadership in theoretical modeling of polymeric liquids and networks, including charged polymers, association, and entanglement effects, and applications to biopolymers, such as mucins."
August 20, 2024	Alexandre Varnek	Herman Skolnik Award, American Chemical Society "The development of chemoinformatics education & training and methodologies for molecular representations and modeling of small molecules & reactions."
June 12, 2024	NSF Center for Molecularly Optimized Networks (<u>Jian Ping Gong</u> and <u>Michael Rubinstein</u> and 17 researchers)	2024 Royal Society of Chemistry Horizon Prize
June 20, 2024	Masumi Tsuda	Women Scientists Award, The 28 th Japanese Association for Molecular Target Therapy of Cancer, "Identification of novel therapeutic drugs targeting glioma stem cells based on glioma niche"
April 17, 2024	Yu Harabuchi	The Young Scientists' Award for 2024 from Japan's Minister of Education, Culture, Sports, Science and Technology, "The creation of quantum chemical computation methods for understanding the photofunctions of molecules"
April 17, 2024	Keisuke Takahashi	The Young Scientists' Award for 2024 from Japan's Minister of Education, Culture, Sports, Science and Technology, "The creation of the field of catalyst informatics and the development of catalytic methane oxidation"

Appendix 2 FY 2024 List of Principal Investigators

NOTE:

*Underline names of principal investigators who belong to an overseas research institution.

*In the case of researcher(s) not listed in the latest report, attach a "Biographical Sketch of a New Principal Investigator"(Appendix 2a).

*Enter the host institution name and the center name in the footer.

<Results at the end of FY2024>							
							Principal Investigators Total: 15
Name	Age	Affiliation (Position title, department, organization)	Academic degree, specialty	Effort (%)*	Starting date of project participation	Status of project participation (Describe in concrete terms)	Contributions by PIs from overseas research institutions
Center Director <u>Satoshi MAEDA</u>	45	Professor, Institute for Chemical Reaction Design and Discovery / Faculty of Science, Hokkaido University	Ph.D., Computational Chemistry	80	October 2018	Usually stays at the center	
Tetsuya TAKETSUGU	60	Professor, Institute for Chemical Reaction Design and Discovery / Faculty of Science, Hokkaido University	Ph.D., Quantum Chemistry	80	October 2018	Usually stays at the center	
<u>Michael RUBINSTEIN</u>	68	Professor, Duke University	Ph.D., Polymer Physics	20	October 2018	- Primarily stays at Partner institution - attends meeting (by online)	- Conducting interdisciplinary research - Recruitment of young researchers
Masaharu YOSHIOKA	56	Professor, Institute for Chemical Reaction Design and Discovery / Graduate School of Information Science and Technology, Hokkaido University	Doctor of Engineering, Knowledge Engineering	50	January 2020	Usually stays at the center	
<u>Alexandre VARNEK</u>	69	Professor, University of Strasbourg	Ph.D., Chemoinform atics	20	October 2018	- Primarily stays at Partner institution - attends meeting (by online)	- Conducting interdisciplinary research - Recruitment of young researchers
Ichigaku TAKIGAWA	48	Specially Appointed Professor, Institute for Chemical Reaction Design and Discovery, Hokkaido University Professor, Graduate School of Frontier Sciences, The University of Tokyo	Ph.D., Machine Learning	20	October 2018	- Primarily stays at Partner institution - attends meeting (by online)	
Tamiki KOMATSUZAKI	60	Professor, Institute for Chemical Reaction Design and Discovery / Research Center of Mathematics for Social Creativity, Research Institute for Electronic Science, Hokkaido University	Ph.D., Mathematical Science	80	October 2018	Usually stays at the center	
Satoru IWATA	56	Specially Appointed Professor, Institute for Chemical Reaction Design and Discovery, Hokkaido University Professor, Graduate School of Information Science and Technology, The University of Tokyo	Doctor of Science, Mathematical Engineering	20	November 2020	- Primarily stays at Partner institution - attends meeting (by online)	
Hajime ITO	57	Professor, Institute for Chemical Reaction Design and Discovery / Faculty of Engineering, Hokkaido University	Doctor of Engineering, Synthetic Chemistry	80	October 2018	Usually stays at the center	
<u>Benjamin LIST</u>	57	Specially Appointed Professor, Institute for Chemical Reaction Design and Discovery, Hokkaido University Professor and Director, Max Planck Institute for Coal Research	Ph.D., Reaction Design	20	October 2018	- Primarily stays at Partner institution - attends meeting (by online)	- Conducting interdisciplinary research - Recruitment of young researchers
Yasuchika HASEGAWA	56	Professor, Institute for Chemical Reaction Design and Discovery / Faculty of Engineering, Hokkaido University	Ph.D., Optical Materials Science	80	October 2018	Usually stays at the center	
Yasuhide INOKUMA	43	Professor, Institute for Chemical Reaction Design and Discovery / Faculty of Engineering, Hokkaido University	Ph.D., Structural Chemistry	80	October 2018	Usually stays at the center	
Jian Ping GONG	63	Professor, Institute for Chemical Reaction Design and Discovery / Faculty of Advanced Life Science, Hokkaido University	Doctor of Science, Doctor of Engineering, Polymer Chemistry	80	October 2018	Usually stays at the center	
Mikako OGAWA	51	Professor, Institute for Chemical Reaction Design and Discovery / Graduate School of Pharmaceutical Sciences, Hokkaido University	Doctor of Pharmaceutic al Sciences, Life sciences	80	April 2023	Usually stays at the center	
Masumi TSUDA	52	Associate Professor, Institute for Chemical Reaction Design and Discovery / Faculty of Medicine, Hokkaido University	Ph.D., Tumor Pathology	80	April 2025	Usually stays at the center	

*Percentage of time that the principal investigator devotes to working for the center vis-à-vis his/her total working hours.

Principal investigators unable to participate in project in FY 2024

Name	Affiliation (Position title, department, organization)	Starting date of project participation	Reasons	Measures taken
Shinya TANAKA	Professor, Faculty of Medicine, Hokkaido University	October 2018	Appointment as Director of the Faculty of Medicine from April 2025.	Masumi TSUDA from the same research group has been appointed as the new PI, while he will continue participating in the project as an ICRéDD Fellow.

Appendix 2a Biographical Sketch of a New Principal Investigator

(within 3 pages per person)

Name (Age) Masumi TSUDA (52)

Affiliation and position (Position title, department, organization, etc.)

Associate Professor

Institute for Chemical Reaction Design and Discovery, Hokkaido University, Japan

Faculty of Medicine, Hokkaido University, Japan

Academic degree and specialty

Ph.D. (Medicine), Hokkaido University

Tumor Pathology

Effort 80 %

* Percentage of time that the principal investigator devote to working for the center vis-à-vis his/her total working hours.

Research and education history

(Research history)

2003.4 – 2003.12 JST Strategic Basic Research Programs (CREST) (Postdoctoral Fellow)

2004.7 – 2006.3 Research Fellow, Memorial Sloan-Kettering Cancer Center (MSKCC), New York, NY, USA

2006.4 – 2014.9 Graduate School of Medicine, Hokkaido University (Assistant Professor)

2014.10 – 2017.5 Same as above (Lecture)

2017.6 – Present Same as above (Associate Professor)

2016.6 – 2017.5 Global Institution for Collaborative Research and Education (GI-CoRE), Hokkaido University
(Lecture)

2017.6 – 2021.3 Same as above (Associate Professor)

2019.2 – 2025.3 Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University

2025.4 – Present Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University
(Associate Professor, Principal Investigator)

(Education history)

1997. 3. School of Health Care Sciences, Faculty of Medicine, Tokyo Medical and Dental University, Bachelor's degree

1999. 3. Graduate School of Env.Earth Science, Hokkaido University, Master's degree

2003. 3. Graduate School of Medicine, Hokkaido University, Ph.D. (Medicine)

Achievements and highlights of past research activities

To date, she has conducted research on cancer, the leading cause of death in Japan, focusing on cancer development (**Proc Natl Acad Sci USA** 2001, CI: 131), proliferation (**Neuro-Oncology** 2014), movement (**Signal Transduct Tar** 2018, IF: 40.8), invasion (**Cell Res** 2009, IF: 28.2), metastasis (**Cancer Sci** 2019), therapy resistance (**Neuro-Oncology** 2014, CI: 134), tumor microenvironment

(**Cancer Res** 2009), drug discovery (**J Am Chem Soc** 2024), etc. A variety of cancer types have been investigated using a lot of experimental techniques, such as include molecular cell biology, biochemistry, pathology, fluorescence bioimaging (**Cell Signal** 2009), protein structure analysis, glycan analysis (**BBA-Gen Subjects** 2022), drug sensitivity testing (**Clin Cancer Res**, 2010), next-generation sequencer gene analysis, scRNAseq, and spatial transcriptome analysis, animal experiments, and clinical specimen verification. In the United States, she performed comprehensive analysis regarding the molecular mechanisms of sarcoma development (**Cancer Res** 2007, CI: 222) and reported the results at a symposium held by the American Cancer Society. She has also conducted several industry-academia collaborative research projects with pharmaceutical companies (**PLoS One** 2016). Since 2012, at GI-CoRE and the WPI-ICReDD research organization at Hokkaido University, she has promoted interdisciplinary research, such as developing cancer stem cell (CSC) creation technology using hydrogels with Gong group (**Adv Funct Mater** 2018; **Adv Healthc Mater** 2021; **Nat Commun** 2022; **ACS Appl Bio Mater** 2025), developing CSC identification method using information science with Komatsuzaki group (**Biochem Biophys Res Commun** 2023), and developing a cancer malignancy evaluation method using Europium complexes with the Hasegawa group (**Sci Rep** 2024). In particular, the development of CSC creation technology using hydrogels (**Nat Biomed Eng.** 2021) has led to progress in the analysis of CSCs that are resistant to treatment in many cancers (**Biochem Biophys Res Commun** 2025a; 2025b; 2025c; 2025d; **Pathol Int.** 2025). On the other hand, she has demonstrated the power of medical pathology in the field of viral infections, another threat to humanity, and conducted analysis of the infection mechanism of influenza viruses (**Nat Commun** 2013) and the pathogenicity of the SARS-CoV-2 (**Nature** 2022a, CI: 331; **Nature** 2022b, CI: 367; **Cell** 2022a, IF: 45.6, CI: 162; **Cell** 2022b, CI: 124; **Cell Host Microbe** 2022; 2024; **Nat Commun** 2023a; 2023b; 2024). She is currently conducting fusion research with ICRReDD List group regarding to develop lipid nanoparticles for use in COVID-19 vaccines.

Through interdisciplinary research at ICRReDD, we will further develop our research toward the eradication of cancer and viral infections, the two major diseases of humanity.

Achievements

(1) International influence * Describe the kind of attributes listed below.

- a) Recipient of international awards : not applicable
- b) Member of a scholarly academy in a major country : not applicable
- c) Guest speaker or chair of related international conference and/or director or honorary member of a major international academic society in the subject field
 1. Tsuda M (2019) Rapid induction of cancer stem cells on double-network hydrogels and therapeutic application. The 10th meeting of Asian Cellular Therapy Organization
 2. Tsuda M (2022) Research development and medical application of cancer stem cells using high-functioning hydrogel. Understanding of Novel Biological Phenomena in Cancer and Immunology Research, (Ree-D International symposium)

- d) Editor of an international academic journal : not applicable
- e) Peer reviewer for an overseas competitive research program (etc.) : not applicable

(2) Receipt of major large-scale competitive funds (over the past 5 years)

(Principal investigator)

1. 2021 – 2023, Grant-in-Aid for Scientific Research (KAKENHI) (B), 21H03802
2. 2024 – 2026, Grant-in-Aid for Scientific Research (KAKENHI) (B), 24K03245

(Co-investigator)

1. 2019 – 2023, Grant-in-Aid for Scientific Research (KAKENHI) (A), 19H01171
2. 2020 – 2022, Grant-in-Aid for Scientific Research (KAKENHI) (C), 20K07441
3. 2021 – 2023, Grant-in-Aid for Scientific Research (KAKENHI) (C), 21K08196
4. 2021 – 2023, Grant-in-Aid for Scientific Research (KAKENHI) (B), 21H03048
5. 2022 – 2024, Grant-in-Aid for Scientific Research (KAKENHI) (B), 23K25172
6. 2022 – 2024, Grant-in-Aid for Scientific Research (KAKENHI) (B), 23K23421
7. 2024 – 2028, Grant-in-Aid for Scientific Research (KAKENHI) (S), 24H00037

(3) Major publications (Titles of major publications, year of publication, journal name, number of citations)

1. Analysis of transforming activity of human synovial sarcoma-associated chimeric protein SYT-SSX1 bound to chromatin remodeling factor hBRM/hSNF2a. 2001, **Proc Natl Acad Sci U S A** (CI: 132)
2. TFE3 fusions activate MET signaling by transcriptional up-regulation, defining another class of tumors as candidates for therapeutic MET inhibition. 2007, **Cancer Res** (CI: 228)
3. A Ca(2+)-dependent signaling circuit regulates influenza A virus internalization and infection. 2013, **Nat Commun.** (CI: 79)
4. Rapid reprogramming of tumour cells into cancer stem cells on double-network hydrogels. 2021, **Nat Biomed Eng.** (CI: 58)
5. Enhanced fusogenicity and pathogenicity of SARS-CoV-2 Delta P681R mutation. 2022, **Nature** (CI: 389)
6. Attenuated fusogenicity and pathogenicity of SARS-CoV-2 Omicron variant. 2022, **Nature** (CI: 453)
7. Virological characteristics of the SARS-CoV-2 Omicron BA.2 spike. 2022, **Cell** (CI: 193)
8. Virological characteristics of the SARS-CoV-2 Omicron BA.2 subvariants including BA.4 and BA.5. 2022, **Cell** (CI: 157)
9. Force-triggered rapid microstructure growth on hydrogel surface for on-demand functions. 2022, **Nat Commun.** (CI: 79)
10. Virological characteristics of the SARS-CoV-2 XBB variant derived from recombination of two Omicron subvariants. 2023, **Nat Commun.** (CI: 165)

(4) Others (Other achievements indicative of the PI's qualification as a top-world researcher, if any.)

- Patent No. 7115749 (Japan), 16/487, 247 (USA): METHOD OF PRODUCING CANCER STEM CELLS

Appendix 3-1 FY 2024 Records of Center Activities

1. Researchers and center staff, satellites, partner institutions

1-1. Number of researchers in the "core" established within the host institution

- Regarding the number of researchers at the Center, fill in the table in Appendix 3-1a.

Special mention

- Enter matters warranting special mention, such as concrete plans for achieving the Center's goals, established schedules for employing main researchers, particularly principal investigators.
- As background to how the Center is working on the global circulation of world's best brains, give good examples, if any, of how career paths are being established for the Center's researchers; that is, from which top-world research institutions do researchers come to the Center and to which research institutions do the Center's researchers go, and how long are their stays at those institutions.

N/A

1-2. Satellites and partner institutions

- List the satellite and partner institutions in the table below.
- Indicate newly added and deleted institutions in the "Notes" column.
- If satellite institutions have been established overseas, describe by satellite the Center's achievements in coauthored papers and researcher exchanges in Appendix 4.

<Satellite institutions>

Institution name	Principal Investigator(s), if any	Notes
N/A	N/A	N/A

< Partner institutions >

Institution name	Principal Investigator(s), if any	Notes
University of Strasbourg	Alexandre Varnek	N/A
Max Planck Institute for Coal Research	Benjamin List	N/A
Duke University	Michael Rubinstein	N/A
ESPCI	-	N/A
Swiss Federal Institute of Technology in Zurich	-	N/A
Peking University	-	N/A
Kyoto University, Graduate School of Informatics	-	N/A
Chubu University, Molecular Catalyst Research Center	-	N/A
The University of Tokyo, Graduate School of Information Science and Technology	Satoru Iwata	N/A
Stockholm University	-	N/A
University of Oslo	-	N/A

1-3. Postdoctoral Positions through Open International Solicitations

- In the columns "number of applications" and "number of selections," put the total number (upper) and the number and percentage of overseas researchers in the < > brackets (lower).

Fiscal year	Number of applications	Number of selections
FY 2024	100	10
	<100, 100%>	<10, 100%>

2. Holding international research meetings

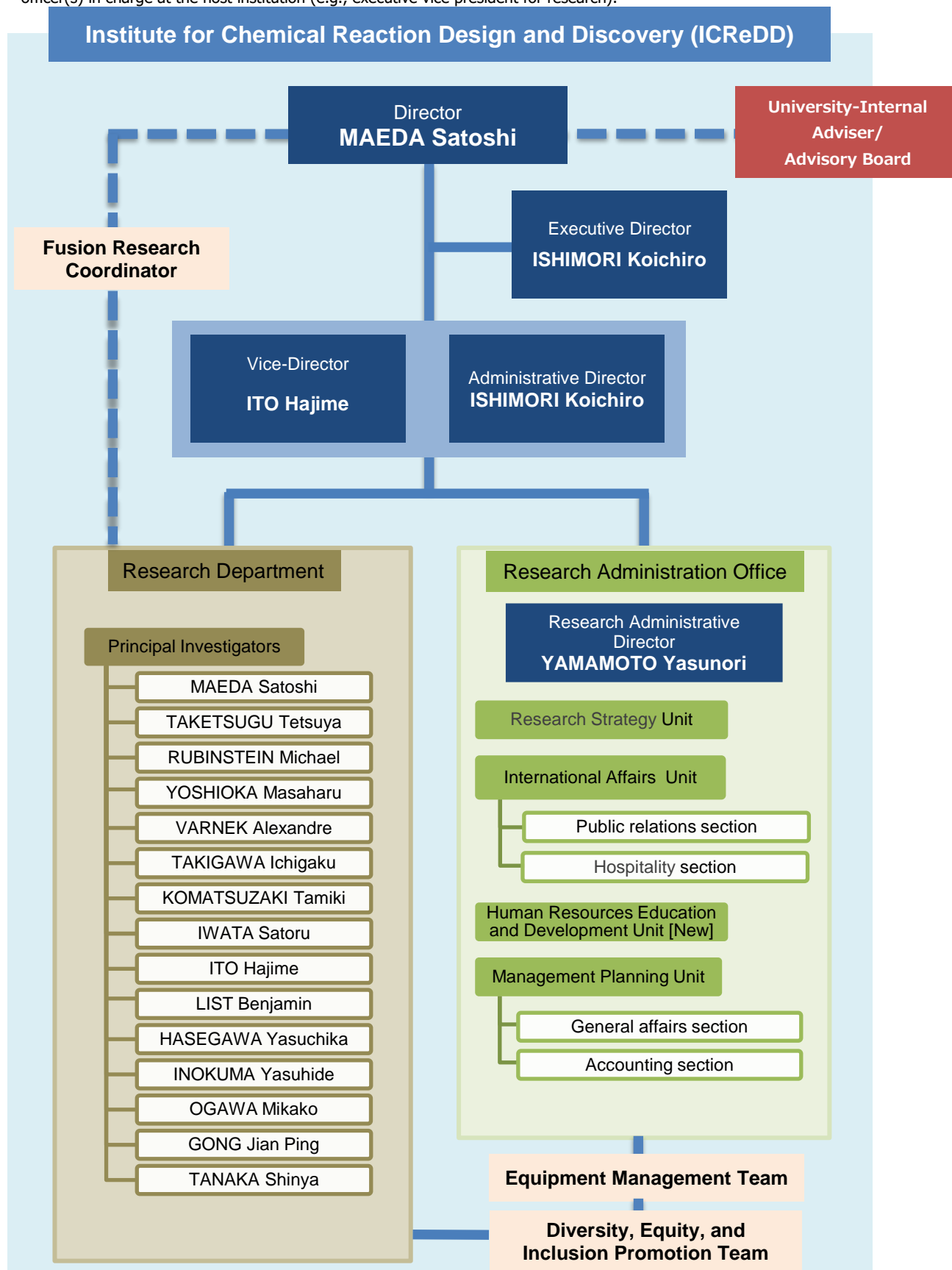
- Indicate the number of international research conferences or symposiums held in FY2024 and give up to three examples of the most

representative ones using the table below.

FY 2024: 3 meetings	Number of participants
Major examples (meeting titles and places held) WPI-SKCM ² & WPI-ICReDD Joint Research Symposium (July 11 th , Hokkaido University, on-site and online)	(Total attendance:114) On-site: 86 From domestic institutions: 70 From overseas institutions: 16 Online: 28 From domestic institutions: 27 From overseas institutions: 1
The 2 nd List Sustainable Digital Transformation Catalyst Collaboration Research Platform Symposium (August 29 th , Hokkaido University, on-site and online)	(Total attendance:78) On-site: 75 From domestic institutions: 73 From overseas institutions: 2 Online: 3 From domestic institutions: 3 From overseas institutions: 0
The 4 th Akira Suzuki Awards Ceremony & the 8 th ICReDD International Symposium + Rising Star Program (October 22 nd -24 th , Hokkaido University, on-site and online)	(Total attendance: 642) On-site: 398 From domestic institutions: 355 From overseas institutions: 43 Online: 244 From domestic institutions: 233 From overseas institutions: 11

3. Diagram of management system

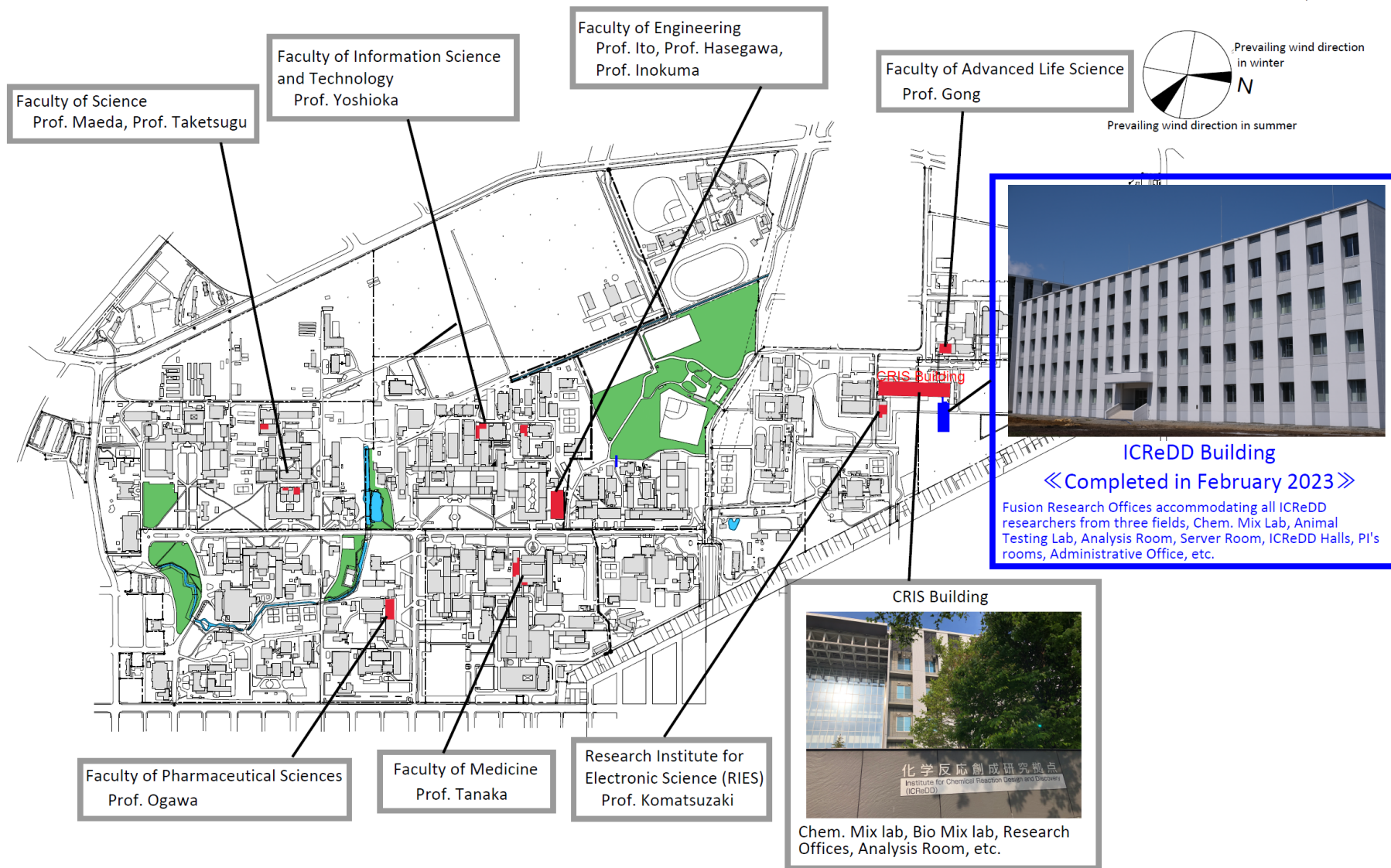
- Diagram the center's management system and its position within the host institution in an easily understood manner.
- If any new changes have been made in the management system from that in the latest "center project" last year, describe them. Especially describe any important changes made in such as the center director, administrative director, head of host institution, and officer(s) in charge at the host institution (e.g., executive vice president for research).



4. Campus Map

- Draw a simple map of the campus showing where the main office and principal investigator(s) are located.

As of March 31, 2025



5. Securing external research funding*

External research funding secured in FY2024

Total: 956,734,899 yen

- Describe external funding warranting special mention. Include the name and total amount of each grant.

* External research funding includes "KAKENHI," funding for "commissioned research projects," "joint research projects," and for others (donations, etc.) as listed under "Research projects" in Appendix 3-2, Project Expenditures.

- Name: Medical Devices Research Results Development Project, AMED
Total Amount: 227,207,500 JPY (acquired by Mikako Ogawa)
- Name: Strategic Basic Research Programs (ERATO), JST
Total Amount: 125,141,200 JPY (acquired by Satoshi Maeda)
- Name: International Leading Research, JSPS
Total Amount: 72,410,000 JPY (acquired by Jian Ping Gong)

Appendix 3-1a FY 2024 Records of Center Activities

Researchers and other center staff

Number of researchers and other center staff

* Fill in the number of researchers and other center staff in the table below.

* Describe the final goals for achieving these numbers and dates when they will be achieved described in the last "center project."

a) Principal Investigators

(full professors, associate professors or other researchers of comparable standing)

(number of persons)

	At the beginning of project	At the end of FY 2024	Final goal (March, 2028)
Researchers from within the host institution	11	12	12
Researchers invited from overseas	3	3	3
Researchers invited from other Japanese institutions	0	0	0
Total principal investigators	14	15	15

b) Total members

	At the beginning of project		At the end of FY 2024		Final goal (March, 2028)	
	Number of persons	%	Number of persons	%	Number of persons	%
Researchers	14	/	79	/	85	/
Overseas researchers	3	21	32	41	38	45
Female researchers	1	7	13	16	21	25
Principal investigators	14	/	15	/	15	/
Overseas PIs	3	21	3	20	7	47
Female PIs	1	7	2	13	2	13
Other researchers	0	/	40	/	45	/
Overseas researchers	0	0	9	23	13	29
Female researchers	0	0	6	15	10	22
Postdocs	0	/	24	/	25	/
Overseas postdocs	0	0	20	83	18	72
Female postdocs	0	0	5	21	9	36
Research support staffs	0	/	2	/	4	/
Administrative staffs	6	/	20	/	19	/
Total number of people who form the "core" of the research center	20	/	101	/	108	/

	At the beginning of project		At the end of FY 2024		Final goal (March, 2028)	
	Number of persons	%	Number of persons	%	Number of persons	%
Doctoral students	67	/	57	/	80	/
Employed	17	25.4	11	19.3	48	60.0

※b) The number of doctoral students in the lower table can be duplicated in the upper table of overall composition.

Appendix 3-2 Project Expenditures

1) Overall project funding

* In the "Total costs" column, enter the total amount of funding required to implement the project, without dividing it into funding sources.

* In the "Amount covered by WPI funding" column, enter the amount covered by WPI within the total amount.

* In the "Personnel," "Project activities," "Travel," and "Equipment" blocks, the items of the "Details" column may be changed to coincide with the project's actual content.

Cost items	Details (For Personnel - Equipment please fill in the breakdown of fiscal expenditure, and the income breakdown for Research projects.)	(Million yens)		Costs (Million yens)
		Total costs	Amount covered by WPI funding	
Personnel	Center Director, Administrative Director, Research Administrative Director	27	12	WPI grant in FY 2024 700
	Principal investigators (no. of persons):9	81	0	
	Full-time faculty members (no. of persons): 7	59	0	
	Part-time faculty members (no. of persons): 16	85	0	
	Specially appointed faculty members (no. of persons): 26	164	164	
	Postdoctoral fellows (no. of persons): 21	84	65	
	Other researchers (no. of persons): 2	8	8	
	Administrative staff (no. of persons): 16	77	31	
	Center allowance	20	20	
	Subtotal	605	300	
Project activities	Startup research project costs	19	19	Costs of establishing and maintaining facilities 0
	Outreach costs	12	11	
	Center operating costs	20	20	
	Environmental improvement costs	20	5	
	Facility rental fees	44	0	
	Utility costs	111	76	
	Public equipments usage fees	5	0	
	Others	68	0	
Subtotal	299	131		
Travel	Domestic travel costs	5	5	Establishing new facilities 0 (Number of facilities: , OO m ²) Repairing facilities 0 (Number of facilities: , OO m ²) Others 0
	Overseas travel costs	26	26	
	Travel cost for scientists on transfer (no. of domestic scientists):3	1	1	
	Subtotal	32	32	
Equipment	Depreciation of equipment	237	237	Costs of equipment procured 237 Automatic Organic Synthesis System (Number of units:1) 151 X-Ray Structural Analysis System (Number of units:1) 27 Others 59
	Subtotal	237	237	
Research projects (Detail items must be fixed)	Project supported by other government subsidies, etc. *1	255	0	
	KAKENHI	261	0	
	Commissioned research projects, etc.	531	0	
	Joint research projects	100	0	
	Others (donations, etc.)	65	0	
Subtotal	1212	0		
Total		2385	700	

*1. Management Expenses Grants (including Management Enhancements Promotion Expenses (機能強化経費)), subsidies etc., indirect funding, and allocations from the university's own resources.

*2 When personnel, travel, equipment (etc.) expenses are covered by KAKENHI or under commissioned research projects or joint research projects, the amounts should be entered in the "Research projects" block.

Appendix 4 FY 2024 Status of Collaboration with Overseas Satellites

1. Coauthored Papers

- List the refereed papers published in FY 2024 that were coauthored between the center's researcher(s) in domestic institution(s) (include satellite institutions) and overseas satellite institution(s). List them by overseas satellite institution in the below blocks.
- Transcribe data in same format as in Appendix 1. Italicize the names of authors affiliated with overseas satellite institutions.
- For reference write the Appendix 1 item number in parentheses after the item number in the blocks below. Let it free, if the paper is published in between Jan.-Mar. 2025 and not described in Appendix 1.

Overseas Satellite 1 **N/A** (Total: 00 papers)

- 1)
- 2)
- 3)
- 4)

Overseas Satellite 2 **N/A** (Total: 00 papers)

- 1)
- 2)
- 3)
- 4)

2. Status of Researcher Exchanges

- Using the below tables, indicate the number and length of researcher exchanges in FY 2024. Enter by institution and length of exchange.

- Write the number of principal investigator visits in the top of each space and the number of other researchers in the bottom.

Overseas Satellite 1:

<To satellite>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2024	N/A	N/A	N/A	N/A	N/A
	N/A	N/A	N/A	N/A	N/A

<From satellite>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2024	N/A	N/A	N/A	N/A	N/A
	N/A	N/A	N/A	N/A	N/A

Overseas Satellite 2:

<To satellite>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2024	N/A	N/A	N/A	N/A	N/A
	N/A	N/A	N/A	N/A	N/A

<From satellite>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2024	N/A	N/A	N/A	N/A	N/A
	N/A	N/A	N/A	N/A	N/A

Appendix 5 FY 2024 Visit Records of Researchers from Abroad

* If researchers have visited/ stayed at the Center, provide information on them in the below table.

* Enter the host institution name and the center name in the footer.

Total: 51

	Name	Age	Affiliation		Academic degree, specialty	Record of research activities (Awards record, etc.)	Time, duration	Summary of activities during stay at center (e.g., participation as principal investigator; short-term stay for joint research; participation in symposium)
			Position title, department, organization	Country				
1	FU, Gregory C.	61	Norman Chandler Professor of Chemistry, Caltech	USA	Ph.D., Organic Chemistry	Noyori Prize of the SSOCJ, Member of the National Academy of Sciences and of the National Academy of Sciences	2024/10/20-10/24 5 days	Participation in the 4th Akira Suzuki Award Ceremony & the 8th ICRéDD International Symposium
2	ASPURU-GUZIŁ, Alán	48	Professor of Chemistry and Computer Science, the University of Tronto	Canada	Ph.D., Computational Chemistry, Quantum Computing	Fellow of the American Association for the Advancement of Science (AAAS), Early Career Award in Theoretical Chemistry	2024/10/21-10/23 3 days	Participation in the 4th Akira Suzuki Award Ceremony & the 8th ICRéDD International Symposium
3	NAUMOV, Panče	49	Professor, New York University Abu Dhabi	UAE	Ph.D., Materials Science	Asian and Oceanian Photochemistry Association Prize, Friedrich Wilhelm Bessel Research Award, Hans and Marlies Zimmer International Scholar Program Award	2024/10/21-10/24 5 days	Participation in the 4th Akira Suzuki Award Ceremony & the 8th ICRéDD International Symposium
4	WATSON, Mary P.	47	Professor, the University of Delaware	USA	Ph.D., Organic Synthesis	Rising Star Award from the Women Chemists' Committee of the American Chemical Society, Delaware ACS Section Award, 2025 Arthur C. Cope Scholar Award	2024/10/20-10/25 6 days	Participation in the 4th Akira Suzuki Award Ceremony & the 8th ICRéDD International Symposium
5	SCHINDLER, Corinna	45	Professor, University of British Columbia	Canada	Ph.D., Organic Chemistry, Metal Catalyst	ACS Pure Chemistry Award, Presidential Early Career Award for Scientists and Engineers, Henry Russel Award (University of Michigan)	2024/10/20-10/25 6 days	Participation in the 4th Akira Suzuki Award Ceremony & the 8th ICRéDD International Symposium
6	AGGARWAL, Varinder Kunar	63	Professor, University of Bristol	UK	Ph.D., Organic Chemistry, Synthetic	Foreign Fellow of the National Academy of Scientists in India, Royal Society Davy Medal, ACS Cope Scholar Award	2024/10/21-10/24 4 days	Participation in the 4th Akira Suzuki Award Ceremony & the 8th ICRéDD International Symposium
7	AHNEMAN, Derek T.	34	IBM Researcher, USA	USA	Ph.D., Scientific AI	Created software for the U. S Food and Drug Administration (FDA)	2024/10/20-10/26 7 days	Participation in the 4th Akira Suzuki Award Ceremony & the 8th ICRéDD International Symposium
8	NAGIB, David A.	40	Professor, College of Arts and Sciences, the Ohio state University	USA	Ph.D., Organic Synthesis	Brown Investigator Award, Merck Outstanding Chemists of Color Award, Arthur C. Cope Scholar Award	2024/10/20-10/25 6 days	Participation in the 4th Akira Suzuki Award Ceremony & the 8th ICRéDD International Symposium
9	YANG, Jeehyun	35	Postdoctoral Fellow, Jet Propulsion Laboratory (JPL)	USA	Ph.D., Physical Chemistry, Kinetic Analysis	Whiteman Fellowship (Massachusetts Institute of Technology), MIT Presidential Fellowship	2024/10/20-10/28 9 days	Participation in the 4th Akira Suzuki Award Ceremony & the 8th ICRéDD International Symposium
10	CRONIN, Leroy	N/A	Professor, University of Glasgow	UK	Ph.D., Artificial Intelligence in Chemistry	RSC Tilden Prize, RISE Award, RSE/BP Hutton Prize, EPSRC Advanced Research Fellow (the University of Versailles)	2024/10/22 1 day	Online participation in the 4th Akira Suzuki Award Ceremony & the 8th ICRéDD International Symposium
11	WATSON, Donald	N/A	Professor, University of Delaware	USA	Ph.D., Organic Synthesis	CAREER Award (the National Science Foundation), Cottrell Scholar Award (the Research Cooperation)	2024/10/24 1 day	Online participation in the 4th Akira Suzuki Award Ceremony & the 8th ICRéDD International Symposium

12	THORAKKATTIL NEERANKUZHYYIL, Mohammed Musthafa	39	Assistant Professor & Head, MES Kalladi College	India	Ph.D. in Chemistry	Conducting research on development of bioactive novel heterocyclic frameworks	2024/8/1-8/30 1 month	Participation in the MANABIYA (Academic) program
13	LIN, Luqing	39	Principal Investigator, School of Chemistry, Dalian University of Technology	China	Ph.D., Pharmaceutical Sciences	Conducting research computational Catalysis for Homogeneous catalysis	2024/7/2-8/23 2 months	Participation in the MANABIYA (Academic) program
14	HE, Yonglin	33	Associate Professor, Renmin University of China	China	Ph.D. in Chemistry	Selected to Young Elite Scientists Sponsorship Program 2024, Wu Yuzhang Young Scholar 2024	2024/6/17-9/2 2.5 months	Participation in the MANABIYA (Academic) program
15	YANG, Hullin	27	Ph.D. student, McGill University	China	Ph.D. student, Philosophy, Department of Chemistry	participated in the writing of a review article published in ChemSusChem	2024/10/28-11/29 1 month	Participation in the MANABIYA (Academic) program
16	WANG, Ting	29	Ph.D. student, Institute of Chemistry, Chinese Academy of Sciences	China	PhD student, Polymer Chemistry and	the preparation anion-exchange membranes (AEMs) with high hydroxide conductivity and alkaline stability	2024/8/26-10/25 2 months	Participation in the MANABIYA (Academic) program
17	HANNARONG, Pitayachinchot	27	Ph.D. candidate, Faculty of Science, Chulalongkorn University	Thailand	PhD. student in Chemical Technology	Awarded a Royal Golden Jubilee (RGJ) Ph.D. Scholarship from the National Research Council of Thailand under the Ministry of Higher Education, Science, Research and Innovation,	2024/5/1-7/31 3 months	Participation in the MANABIYA (Academic) program
18	DE SILVA, Nuwan	46	Associate Professor, Western New England University	USA	Associate Professor of Chemistry	the WNE Academic Inventor Award, Tennessee Tech University Graduate Teaching Assistant Award, ISU Research Excellence Award, Ames Laboratory Inventor Incentive Award, Nominations for the Teaching Excellence Award in 2019, 2022, and 2024, and achieved tenure and promotion to Associate Professor of Chemistry in 2022.	2024/8/19-11/11 3 months	Participation in the MANABIYA (Academic) program
19	CSOMOS, Attila	27	Ph.D. student, Eötvös Loránd University	Hungary	Ph.D. student, Organic Chemistry+	ELTE TDK Conference (2nd prize), ELTE TDK Conference (1st prize, special prize by EGIS), OTDK Conference (2nd prize), Niveau prize for the best thesis work by the Asso. of Hungarian Chemists (MKE), Zechmeister László Prize 1st place (by MTA Chemical Biology committee)2022, Scholarship of the Association of Hungarian American Academics (2000 USD grant)2022	2025/1/6-2/7 1 month	Participation in the MANABIYA (Academic) program
20	DE SILVA, Chamila	48	Assistant Professor, Springfield College	USA	Ph.D. in Physical Chemistry	The Iowa State University Teaching Excellence Award in 2012 and the Howard Hughes Medical Institute Teaching Fellow in 2013.	2024/8/19-11/11 3 months	Participation in the MANABIYA (Academic) program
21	KIM, Namhee	26	Integrated M.S.-Ph.D. student, Yonsei University	Korea	Integrated M.S.-Ph.D. Chemistry	Outstanding Teaching Assistant Award, Department of Chemistry, Yonsei University, Outstanding Poster Award, The Polymer Society of Korea	2024/5/21-8/9 2.5 months	Participation in the MANABIYA (Academic) program
22	KOVACS, Ervin	40	Research Fellow, Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences	Hungary	Ph.D., Organic Chemistry and Technology	Postdoctoral Excellence Grant (OTKA-PD by NKFIH, Hungary), 1st Prize in Chemical Calculation (Organized by BME Szent-Györgyi Albert Student's Association), Research Prize of Centenary Foundation of Gedeon Richter Plc., Földi Zoltán Award), 2nd prize with team Knock Nevis at Freshhh2008 Competition, Conference Award (2nd prize) of Chemistry Collegium Conference, Organic Chemistry Section	2024/8/13-9/20 1 month	Participation in the MANABIYA (Academic) program
23	THAMMANATPONG, Kittimeth	25	Ph.D. student, Mahidol University	Thailand	Ph.D. student, computational chemistry	Conducting research on Theoretical and Computational Chemistry	2024/11/1-2025/1/24 3 months	Participation in the MANABIYA (Academic) program

24	HEMINGWAY, Jack	27	Postdoctoral Research Associate, School of Natural and Environmental Sciences, Newcastle University	UK	PhD, Predicting and Tailoring Properties of Energetic Materials	Conducting research on Computational Chemistry	2024/7/8-9/6 2 months	Participation in the MANABIYA (Academic) program
25	LOWE, Matthew	23	Ph.D. student, School of Natural and Environmental Sciences, Newcastle University	UK	Ph.D. student, field of mechanochemistry	Conducting research on Synthesis and reactivity of organosodium compounds via mechanochemistry.	2024/9/11-11/11 2 months	Participation in the MANABIYA (Academic) program
26	GODEC, Nejc	24	M2 student, University of Strasbourg	Slovenia	M2 student, Chemoinformatics	French/Slovenian Double Master's Degree in Chemistry and Chemoinformatics, Erasmus exchange - bachelor thesis research	2025/2/3-5/30 4 months	Participation in the MANABIYA (Academic) program
27	LI, Christina M.	37	Associate Professor, Purdue University	USA	Ph.D., Inorganic Chemistry, Materials Chemistry	Career Award, Outstanding Contributions to Teaching by Assistant Professor, Seeds for Success Award	2024/5/19 1 day	Participation in the ICRéDD International Seminar <i>*Invitation of Overseas Researchers, etc. to ICRéDD</i>
28	UYEDA, Christopher H.	41	Professor, Purdue University	USA	Ph.D., Organometallic Chemistry	Camille Dreyfus Teacher-Scholar Award, Kavli Fellow, Lilly Grantee Award	2024/5/10 1 day	Participation in the ICRéDD International Seminar
29	MALKINA, Olga L.	N/A	Slovak Academy of Sciences	Slovakia	Ph.D., Computational Chemistry	Program founder of ReSpec, a computer simulation program to predict and understand molecular and material properties from DFT calculations.	2024/6/26 1 day	Participation in the ICRéDD International Seminar
30	MALKIN, Vladimir G.	N/A	Slovak Academy of Sciences	Slovakia	Ph.D., Computational Chemistry	International Organization Committee member of the 8th Japan-Czech-Slovakia (JCS) International Symposium on Theoretical Chemistry	2024/6/26 1 day	Participation in the ICRéDD International Seminar
31	MUSAEV, Djamaladdin G.	N/A	Professor, Emory University	USA	Ph.D., Computational and Theoretical	Japan Society for Promotion of Science (JSPS) Senior Fellowship, Member of the Catalysis Innovation Consortium	2024/7/14 1 day	Participation in the ICRéDD International Seminar
32	KIM, Byeong-Su	49	Professor, Yonsei University	Korea	Ph.D., Nanotechnology	Outstanding Teaching Award (Yonsei University), Sigma-Aldrich Chemist Award (the Korean Chemical Society)	2024/7/22 1 day	Participation in the ICRéDD International Seminar
33	EISENSTEIN, Odile	75	Emeritus Professor, ICGM (Institut Charles Gerhardt Montpellier)	France	Ph.D., Computational Chemistry	Member of the French Academy of Sciences, Member of the US National Academy of Sciences	2024/8/21, 26, 29 3 days	Participation in the ICRéDD International Seminar <i>*Invitation of Overseas Researchers, etc. to ICRéDD</i>
34	CHO, Seung Hwan	41	Professor, POSTECH	Korea	Ph.D., Chemistry	POSTECH Young Distinguished Professor, Toray Research Grant for Young Investigator	2024/10/4 1 day	Participation in the ICRéDD International Seminar
35	WALES, David	61	Professor of Chemical Physics, the University of Cambridge	UK	Ph.D., Biological Chemistry	ICReDD Award 2020, Visiting Miller Professorship (the University of California, Berkeley)	2024/11/21-11/25 6 day	Participation in the ICRéDD International Seminar <i>*Invitation of Overseas Researchers, etc. to ICRéDD</i>
36	FORBES, Malcolm D.E.	N/A	Professor, Bowling Green State University	USA	Ph.D., Physical Organic Chemistry	Co-Chair of the 2015 GRC on Photochemistry, President of the Inter-American Photochemical Society	2024/12/3 1 day	Participation in the ICRéDD International Seminar
37	REDDY, C. Malla	50	Professor, Indian Institute of Technology	India	Ph.D., Crystal Engineering	Prestigious Swarna Jayanti fellowship by the Department of Science and Technology (Government of India)	2024/12/12 1 day	Participation in the FCC-ICReDD International Seminar
38	SKIPPER, Magdalena	55	Editor-in-Chief of the journal <i>Nature</i>	UK	Ph.D., Genetics	Appointed as the first female editor of <i>Nature</i>	2025/2/10 1 day	Participation in the ICRéDD International Seminar

39	ROBERT, Vincent	55	Professor, University of Strasbourg	France	Ph.D., Chemical Physics	Director of the Institut de Chimie de Strasbourg, UMR7177 CNRS/University of Strasbourg	2025/3/12 1 day	Participation in the ICREDD International Seminar
40	YUDIN, K. Andrei	55	Professor, University of Toronto	Canada	Ph.D., Chemistry	Canada Research Chair in Medicine by Design at the University of Toronto	2024/6/11-6/18, 7/4-7/9 14 days	Participation in the ICREDD International Seminar *Invitation of Overseas Researchers, etc. to ICREDD
41	SCHNERMANN, J. Martin	N/A	Senior Investigator, Center for Cancer Research, National Cancer Institute	USA	Ph.D., Chemical Biology	Senior Investigator, Center for Cancer Research, National Cancer Institute	2024/5/20 1 day	Participation in the ICREDD International Seminar *Invitation of Overseas Researchers, etc. to ICREDD
42	MEYER Ulrich	N/A	Science Editor, Mayer Scientific Editing	Germany	Ph.D., Chemistry	Science Editor, Mayer Scientific Editing	2024/5/30 1 day	Participation in the ICREDD International Seminar *Invitation of Overseas Researchers, etc. to ICREDD
43	HSU, Shan-hui	N/A	Distinguished Professor, National Taiwan University	Taiwan	Ph.D., Polymer Science and Engineering	Distinguished Professor, National Taiwan University	2024/7/30 1 day	Discussions for future collaboration
44	LIAO, Chao-Yaug	N/A	Associated Professor, National Central University	Taiwan	Ph.D., Mechanical Engineering	Associated Professor, National Central University	2024/7/30 1 day	Discussions for future collaboration
45	CHANG, Shu-Wei	N/A	Professor, National Taiwan University	Taiwan	Ph.D., Civil Engineering	2024 NSTC Ta-You We Memorial Award, 2022 Young Investigator Award, Asian Pacific Association for Computational Mechanics (APACM), 2022 Young Scholar Award, Society of Theoretical and Applied Mechanics of the Republic of China	2024/7/30 1 day	Discussions for future collaboration
46	Chen, LING	N/A	Assistant Professor, National Yang Ming Chiao Tung University	Taiwan	Ph.D., Computer Science	Richard Jago Memorial Prize 2024, Sponsorship for attending the 2014 C9-Go8 Forum on Global challenges of Ageing Populations, Sydney and The 2014 Premier's Awards for Open Data - the Best Use of Open Data Award and Microsoft startup Q Award	2024/7/30 1 day	Discussions for future collaboration
47	WANG, Chih-Chieh	N/A	Professor, National Yang Ming Chiao Tung University	Taiwan	Ph.D., Engineering	Best Paper Award, the 27th International Conference on Technologies and Applications of Artificial Intelligence (TAAI 2022)	2024/7/30 1 day	Discussions for future collaboration
48	RUBINSTEIN, Michael	67	Principal Investigator at ICREDD, Professor at Duke University	USA	Ph.D., Polymer Physics	2025 ACS Award in Polymer Chemistry from the American Chemical Society, 2018 Bingham Medal	2024/8/25-8/30 6 days	Visit as a principal investigator, participation in the ICREDD Site Visit 2024
49	GUO, Hao	29	Postdoctoral Associate, Duke University	USA	Ph.D., Molecular Modeling and Simulation	Conducting computational and theoretical research in Polymer Physics	2024/8/26-9/6 11 days	Visit as a co-researcher, participation in the ICREDD International Seminar
50	VARNEK, Alexandre	68	Principal Investigator at ICREDD, Professor at University of Strasbourg	USA	Ph.D., Chemoinformatics	2024 Herman Skolnik Award	2024/8/25-8/30 6 days	Visit as a principal investigator, participation in the ICREDD Site Visit 2024
51	LIST, Benjamin	57	Principal Investigator & Professor, ICREDD, Director & Professor, Max-Planck-Institut fuer Kohlenforschung	Germany	Ph.D., Chemical Synthesis and Catalysis	The Nobel Prize in Chemistry, Herbert C. Brown Award 2022 for Creative Research in Synthetic Methods, Member of the German National Academy of Science Leopoldina	2024/8/25-9/2 8 days	Visit as a principal investigator, giving a lecture in the ICREDD Site Visit 2024 and 2nd symposium for the List Sustainable Digital Transformation Catalyst Collaboration Research Platform

Appendix 6 FY2024 State of Outreach Activities

* Fill in the numbers of activities and times held during FY2024 by each activity.

* Describe the outreach activities in the "6. Others" of Progress Report, including those stated below that warrant special mention.

Activities	FY2024 (number of activities, times held)
PR brochure, pamphlet	4: Monthly post card J/E, Quarterly news poster and newspaper J/E, Annual report J/E, MANABIYA pamphlet (E)
Lectures, seminars for general public	2: -Lecture on a machine learning model to identify features of crystals by Assist. Prof. Ide (June 8 th , 2024) -Seminar series for high school teachers (8) "The WPI's latest research" (July 23rd, 2024 [Hosted with I ² CNER])
Teaching, experiments, training for elementary, secondary and high school students	3: -ICReDD's 3 laboratories participated in "Dream Chemistry 21" program of the Hokkaido Branch of the Chemical Society of Japan (Hands-on lab experience for high school students, Aug. 1-2 nd , 2024), - "Academic Fantasista" (Lecture and lab tour for high school students by Assoc. Prof. Harabuchi, Oct. 8 th) - "Academic Fantasista" (the same as above, Dec. 17 th)
Open houses	1: Joint open campus event (June 8 th , 2024)
Participating, exhibiting in events	1: Exhibition booth (The 13 th WPI Science Symposium, Nov. 16 th , 2024)
Press releases	8: Press releases (research)
Others (Research News Articles on ICRReDD Web)	6
Others (SNS)	6: X, Facebook, YouTube, Instagram (E), Instagram (J), LinkedIn
Others (ICReDD Goods)	5: Tote bag, Sacoche, File folder, Pin badges, Stuffed toy keychain

*If there are any rows on activities the center didn't implement, delete that (those) row(s). If you have any activities other than the items stated above, fill in the space between parentheses after "Others" on the bottom with the name of those activities and state the numbers of activities and times held in the space on the right. A row of "Others" can be added, if needed.

Outreach Activities and Their Results

List up to three of the Center's outreach activities carried out in FY 2024 that have contributed to enhancing the brand or recognition of your Center and/or the brand of the overall WPI program, and describe its concrete contents and effect in narrative style. (Where possible, indicate the results in concrete numbers.)

Examples:

- As a result of using a new OO press-release method, a OO% increase in media coverage was obtained over the previous year.
- By holding seminars for the public that include people from industry, requests for joint research were received from companies.
- We changed our public relations media. As a resulting of using OO to disseminate information, a OO% increase in inquiries from researchers was obtained over the previous year.
- As a result of vigorously carrying out OO outreach activity, ¥OO in external funding was acquired.

1) In FY2024, the ICRReDD International Symposium and the "Rising Star Program", which are originally two independent events, were jointly held as a large three-day symposium. ICRReDD invited a wide range of presenters from Japan and abroad, with the privilege of supporting travel expenses for the best students among the poster presentation applicants. The total number of presenters was 52 (39 students and 13 researchers), of which 2 students from Japan and 1 student from Thailand were supported with travel expenses. The breakdown of the 52 presenters' affiliations is: 36 from Hokkaido University, 8 from other domestic institutions, and 8 from four foreign institutions. The total number of presenters increased by 2.4 times (57% increase) and the total number of participating countries increased from 3 to 5, as 22 (19 from Hokkaido University, 1 from another domestic institution, and 2 from 2 foreign countries) presented posters in the previous year's Rising Star Program.

2) The MANABIYA page on the ICRReDD website was reorganized and enhanced. In addition, a new pamphlet summarizing the MANABIYA application process was published and distributed at events and to visitors. As a result, 50 applications were received for the 2025 MANABIYA program, which was solicited in FY2024, a 1.7-fold increase (42% increase) over the 29 applications received in the previous year.

3) Continuing from the previous year, Associate Professor Yu Harabuchi's project was selected for "Academic Fantasista," a research

support program conducted by Hokkaido University in cooperation with the Hokkaido Shimbun to promote "science and technology dialogue with the public," and through this program he gave classes and facility tours to two high schools in Hokkaido. One of the schools requested to participate in the next year's program, and we plan to continue this activity.

Appendix 7 FY 2024 List of Project's Media Coverage

* List and describe media coverage (e.g., articles published, programs aired) in FY2024.

* Enter the host institution name and the center name in the footer.

1) Japan

	Date	Types of Media (e.g., newspaper, magazine, television)	Description
1	2024/4/12	Newspaper	Feature article on "the machine learning model to identify features of crystals" by PI. Inokuma group and PI.Takigawa group, Asahi Shimbun
2	2024/4/26	Newspaper	Article on the research press release about "Generalized Transition Moment and Oscillator Strength for Optimal Control of Excited States using Near-Field Light" by Assist. Prof. Iwasa, Nikkei Press Release
3	2024/7/15	Newspaper	Feature article on Hokkaido University's Sustainable Campus Management Plan, introducing the ICRéDD building, Hokkaido Shimbun
4	2024/8/23	Magazine	Feature article on the scientific career of Prof. Maeda, "Front Runner", No. 152", Nikkei Science
5	2024/8/29	Newspaper	Article on the donation ceremony of the Nobel Prize medal replica from Prof. List, Hokkaido Shimbun
6	2024/8/31	Newspaper	Article on the donation ceremony of the Nobel Prize medal replica from Prof. List, Yomiuri Shimbun
7	2024/9/5	Newspaper	Article on the donation ceremony of the Nobel Prize medal replica from Prof. List, Mainichi Shimbun
8	2024/10/8	Newspaper	Feature article on the Nobel Prizes 2024, mentioning the topics of Prof. List's Nobel Prize 2021 in chemistry and the Nobel Prize medal replica donation ceremony at HU, Hokkaido Shimbun
9	2024/11/5	Newspaper	Digest version of the feature article on the biography of Prof. Maeda, "Front Runner", No. 152" on Nikkei Science, NIKKEI Shimbun online
10	2024/11/25	Newspaper	Feature article on the research press release on "Virtual Ligand-Assisted Optimization: A Rational Strategy for Ligand Engineering", by PIs Maeda and Iwata group, NIKKEI Shimbun
11	2024/12/18	Newspaper	Feature article on the work of Pathologists with commentary by Prof. Tanaka, Hokkaido Shimbun
12	2025/2/27	Newspaper	Article on the research press release on "Rapid self-strengthening in double network hydrogels triggered by bond scission" by Gong group, Nikkan Kogyo Shimbun
13	2025/2/28	Online news	Article on the research press release on "Rapid self-strengthening in double network hydrogels triggered by bond scission" by Gong group, fabcross for Engineer

14	2025/3/2	Online news	Article on the research press release on "Rapid self-strengthening in double network hydrogels triggered by bond scission" by Gong group, Newswitch (by Nikkan Kogyo Shimbun)
15	2025/3/24	Newspaper	Feature article on the scientific career of Prof. Inokuma, "Science Human", Yomiuri Shimbun

2) Overseas

	Date	Types of Media (e.g., newspaper, magazine, television)	Description
1	2024/11/30	Online News	Article on ICRéDD research press release (EN): "A holy grail found for catalytic alkane activation"; Chemical Processing; https://www.chemicalprocessing.com/processing-equipment/reaction-synthesis/news/55246489/alkanes-activate-form-of-a-new-catalytic-method
2	2024/11/11	Online News	Article on ICRéDD research press release (EN): "A holy grail found for catalytic alkane activation"; hydrocarbononline.com; https://www.hydrocarbononline.com/doc/a-holy-grail-found-for-catalytic-alkane-activation-0001
3	2024/10/16	Online News	Article on ICRéDD research press release (EN): "A holy grail found for catalytic alkane activation"; 360doc个人图书馆; http://www.360doc.com/content/24/1015/10/71227952_1136603029.shtml
4	2024/10/15	Online News	Article on ICRéDD research press release (EN): "A holy grail found for catalytic alkane activation"; Chip.pl; https://www.chip.pl/2024/10/rewolucyjne-katalizatory-reakcje-chemiczne
5	2024/10/15	Online News	Article on ICRéDD research press release (EN): "A holy grail found for catalytic alkane activation"; 科普中国; https://cloud.kepuchina.cn/newSearch/imgText?id=7245472989077778432
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