The CATALYST

Helping you react with chemical reactions

Issue 18
December 2024

What is a reaction in the first place?

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

What is a reaction in the first place?

Thank you for reading and we are looking forward to your continued patronage. This is CATALYST issue 18. We have covered a variety of topics thus far and would like to touch on "What is a reaction?" again here. In this issue, we will discuss organic chemical reactions and synthetic organic chemistry.

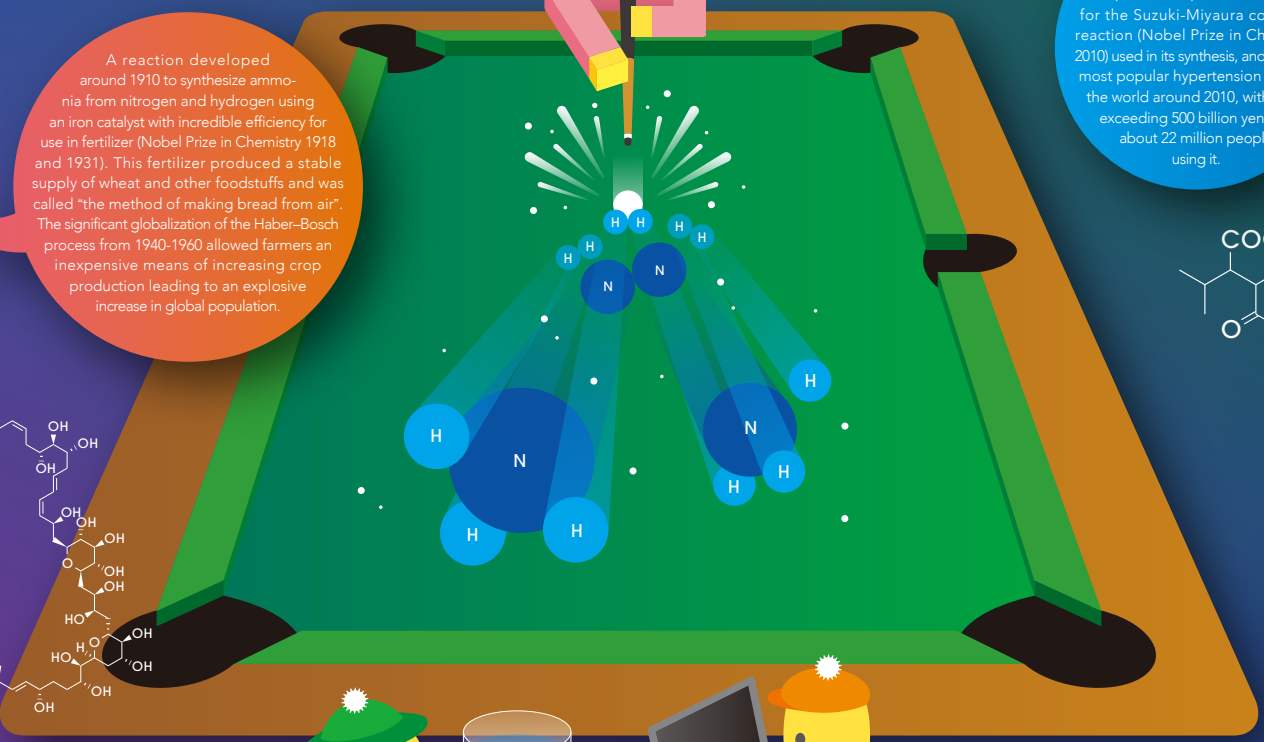
Haber–Bosch process

$$3H_2 + N_2 \rightarrow 2NH_3$$

A reaction developed around 1910 to synthesize ammonia from nitrogen and hydrogen using an iron catalyst with incredible efficiency for use in fertilizer (Nobel Prize in Chemistry 1918 and 1931). This fertilizer produced a stable supply of wheat and other foodstuffs and was called "the method of making bread from air". The significant globalization of the Haber–Bosch process from 1940-1960 allowed farmers an inexpensive means of increasing crop production leading to an explosive increase in global population.

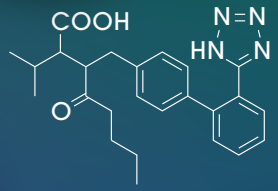
Synthetic Chemist

Synthesize organic molecules using a variety of chemical reactions.

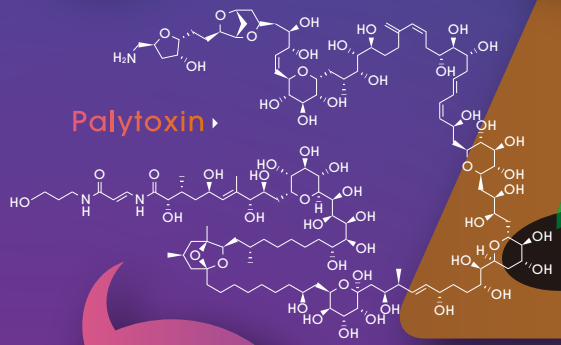


A drug for hypertension developed by Novartis AG (Switzerland). It is also famous for the Suzuki-Miyaura coupling reaction (Nobel Prize in Chemistry 2010) used in its synthesis, and was the most popular hypertension drug in the world around 2010, with sales exceeding 500 billion yen and about 22 million people using it.

Valsartan



Palytoxin



A potent toxin discovered in Hawaiian sea anemones. Its huge and complex molecular structure attracted the attention of chemists around the world, and its total synthesis was achieved by Professor Kishi at Harvard University in 1994. The Suzuki-Miyaura coupling reaction was used as a key part of the synthesis and made the name famous.

Paclitaxel, a natural product isolated from the bark of the Pacific yew tree, was structurally determined in 1971 and has been synthesized within 34-60 reactions by 11 groups over 30 years of research beginning in 1994. It shows remarkable anti-tumor activity and is widely used as an anti-cancer drug for the treatment of breast cancer, ovarian cancer, and lung cancer.

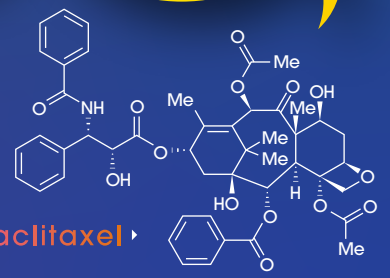
Bioorganic Chemist

Extract organic molecules from nature and study their molecular structure and function.

Reaction Development Chemist

Researching new organic chemical reactions for use in synthesis

Paclitaxel



1. Atoms, elements, molecules, chemical bonds, chemical reactions

Before we discuss chemical reactions, let's review atoms and molecules. The atom is the smallest unit of matter represented in the periodic table. An atom has the same number of protons and electrons as its atomic number. Elements are types of atoms and are classified into "metallic elements" and "non-metallic elements" in the periodic table. Molecules are composed of two or more atoms attached to each other by chemical bonds. Types of chemical bonds include covalent bonds, ionic bonds, and metallic bonds. In a covalent bond, non-metallic elements share electrons with each other to form electron pairs. An ionic bond is a bond between a metallic element and a non-metallic element however, rather than sharing, the metallic element gives an electron to the non-metallic element creating a positive charge on the metallic element and a negative charge on the non-metallic element. Metallic bonds occur between metallic elements sharing a "cloud" of electrons. A chemical reaction is the process of recombining chemical bonds between molecules to form new molecules.

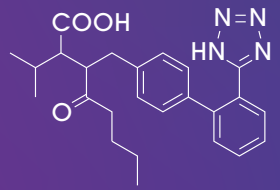
2. About organic chemistry

The field of organic chemistry covers molecules consisting primarily of hydrogen, carbon, nitrogen, oxygen, and halogen elements. The number of bonds an atom can form depends on the element. For example, carbon likes to form 4 bonds, nitrogen forms 3 bonds, oxygen forms 2 bonds, and hydrogen and halogens form 1 bond. These aspects provide a foundation from which an infinite number of molecules can be created and studied. Nature itself, through plants and animals, synthesizes complex molecules (natural products) that can be extracted and studied for medicine, materials, and more. Through reaction development, the study of new chemical reactions, organic chemists have created an intricate synthetic toolbox for accessing new natural products and molecules inaccessible by Nature itself. With growing technology, other fields of research, such as inorganic chemistry, theoretical chemistry, physics, biology, and more, can be integrated into organic chemistry, growing the field with interesting complexity.

3. Organic chemical reactions (Synthetic organic chemistry)

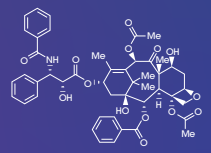
An organic chemical reaction is a recombination of molecules in which chemical bonds within an organic molecule are broken or new chemical bonds are formed. Following the law of conservation of mass, the number of atoms does not change before and after a chemical reaction. The mass of reactants is the same as the mass of the products. Synthetic organic chemistry, the chemistry of synthesizing organic molecules, is the basis of manufacturing. It has been used to synthesize a wide variety of molecules needed by humankind. These include natural products, pharmaceuticals, pesticides, polymers such as plastics, rubber, cellulose, proteins, and genes, and organic materials such as fats, oils, surfactants, liquid crystals, organic LEDs, and organic solar cells. Organic synthesis has been described as an art, requiring heightened creativity and intuition along with knowledge of chemical principles to perform complex molecular reactions.

Valsartan



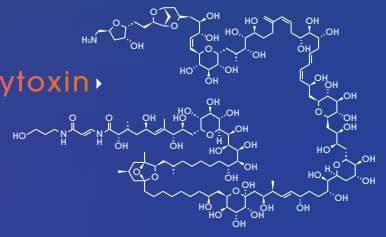
4. Historical examples of synthetic organic chemistry

Total synthesis is a specialization within organic chemistry focused on constructing complex organic molecules, often natural products, using chemical reactions. Natural products are extracted from nature and their molecular structures can be elucidated using various analytical instruments. With knowledge of the molecular structure, a methodology is designed to synthesize the desired molecule from small organic molecules using a series of chemical reactions. Development of natural product synthesis is critical as the extraction of natural products can be expensive and low yielding for research use, as was the case with Palytoxin ($C_{129}H_{223}N_3O_{54}$, molecular weight 2680) and Paclitaxel ($C_{47}H_{51}NO_{14}$, molecular weight 854). The fusion of chemical reactions with the latest technologies, such as simulation and AI, has contributed towards environmentally friendly manufacturing, including the effective use of limited resources and the reuse of waste materials.



Paclitaxel

Palytoxin



Activation!

Quiz

Once the structure of an organic molecule is known, the molecule can be synthesized using ____.

- A adhesives
- B 3D printers
- C organic chemical reactions
- D a microscope

Send us your answer!

Check our Instagram highlights for the answer to the quiz!
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ICReDD News

December 2024

New Researchers

Taihei Oki
Combinatorial Optimization and Mathematical Engineering in Computational Chemistry

Julong Jiang
Mechanochemical Reactions using AFIR method

Pingyu Jiang
Amphidynamic crystalline materials with Photo-Functions

Selected Publications (from September 2024 to November 2024)

A holy grail found for catalytic alkane activation

(Ravindra K. Raut, Satoshi Maeda, Nobuya Tsuji, Benjamin List)

https://www.icredd.hokudai.ac.jp/research/12556

Achieving the Construction of Diverse Small-Molecule Frameworks Using Cobalt Catalysts

(Tsuyoshi Mita, Satoshi Maeda)

https://www.icredd.hokudai.ac.jp/research/12543

Control of Hydride Content and High-Precision Prediction for Perovskite Oxyhydride Using Image-Based Machine Learning System

(Yuki Ide, Ichigaku Takigawa, Yasuhide Inokuma)

https://www.icredd.hokudai.ac.jp/research/12600

Mechanistic Exploration of *N*-Heterocyclic Carbene Boranes as the Hydrogen Atom Transfer Reagent in Selective Hydrodefluorination Reactions

(Amit K. Jaiswal, Satoshi Maeda, Dennis Chung-Yang Huang)

https://www.icredd.hokudai.ac.jp/research/12665

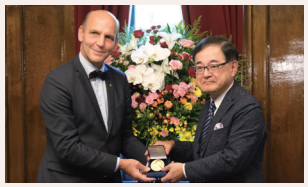
New method improves ligand design for chemical reactions

(Wataru Matsuoka, Taihei Oki, Yu Harabuchi, Satoru Iwata, Satoshi Maeda)

https://www.icredd.hokudai.ac.jp/research/12645

Event

- Donation Ceremony for Nobel Prize Medal Replica (Aug. 28)
- The 2nd List Platform Symposium (Aug. 29)
- The 4th Akira Suzuki Awards Ceremony & the 8th ICReDD International Symposium + Rising Star Program (Oct. 22-24)
- The 13th WPI Science Symposium "The world expands through science" (Nov. 16)

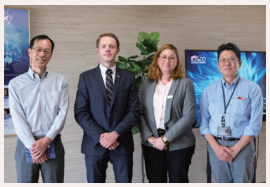


Donation Ceremony for Nobel Prize Medal Replica

The 4th Akira Suzuki Award Ceremony & the 8th ICReDD International Symposium + Rising Star Program

Visitor

- A delegation led by Dr. Adelaine Lassaux, Scientific Attachée, Ambassade de France au Japon (Sep. 18)
- Yasuhiro Awatsuji, analyst, Science and Technology Policy Bureau, MEXT (Oct. 10)
- The Fukushima Institute for Research, Education and Innovation (F-REI) (Nov. 28)

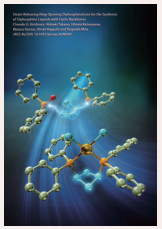


A delegation led by Dr. Adelaine Lassaux, Scientific Atttachée, Ambassade de France

Outreach

- Monthly Research Postcard
- The CATALYST Issue 17
- MANABIYA Pamphlet

The CATALYST 17th Issue



Monthly Research Postcard

Award

- The Chemist Award BCA 2024 (Kubota)

Researcher Profile

vol.18

Dennis Chung-Yang Huang

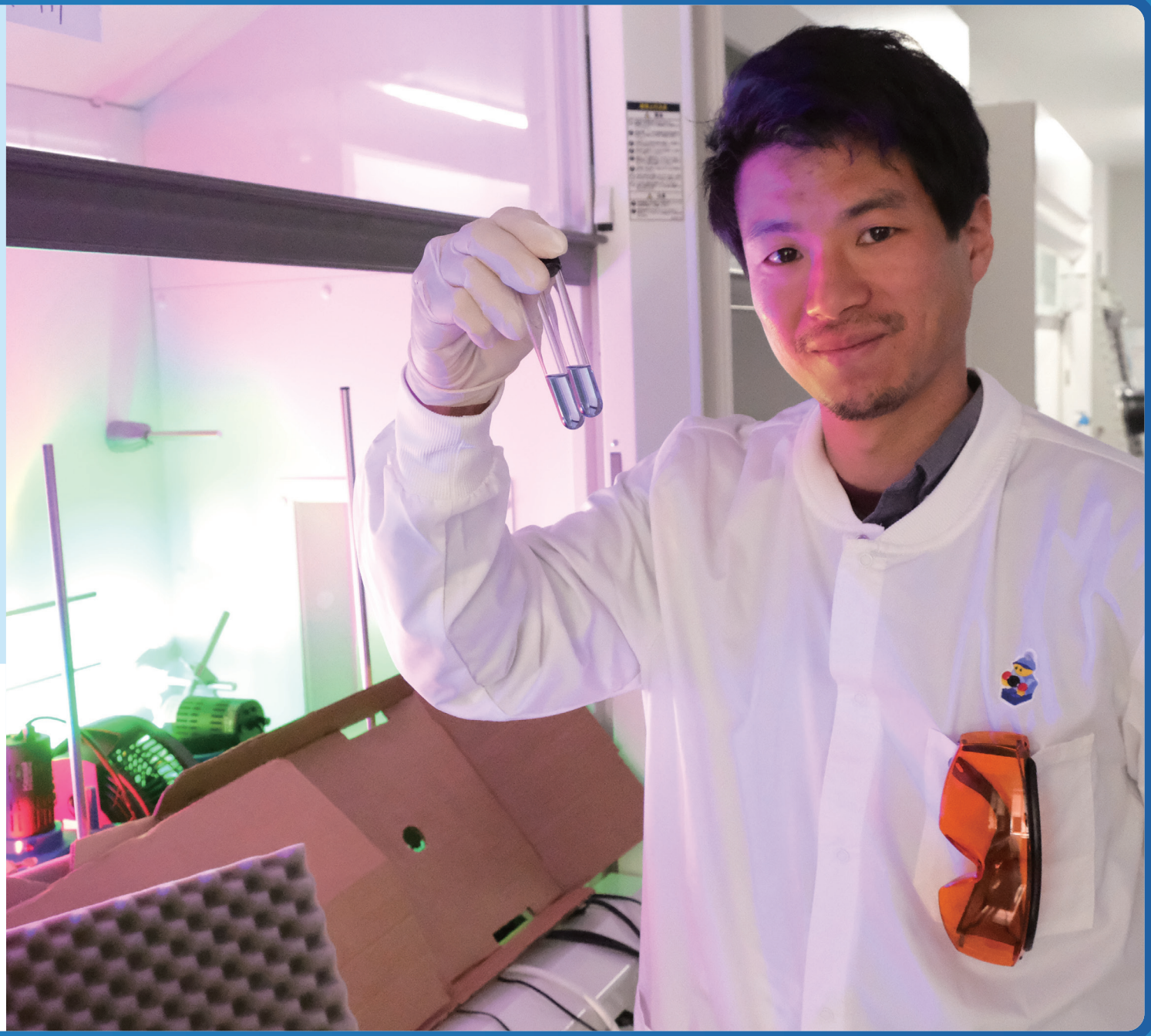
The research in our lab focuses on developing new chemical reactions to construct molecular structures with intriguing properties. We are particularly interested in leveraging light and metal catalysts to drive these transformations. Additionally, we incorporate computational and data science approaches to accelerate reaction development and gain deeper mechanistic insights.

Representative Papers:

ACS Catal. 2024, 14, 17547–17555.
J. Am. Chem. Soc. 2024, 146, 21367–21376.
Chem. Sci. 2023, 14, 2482–2488.

Short Biography

Born and raised in Taiwan, Dennis moved to the United States after high school to complete his bachelor's degree at the Massachusetts Institute of Technology in 2010. He subsequently earned his PhD from Princeton University under the guidance of Prof. Abigail Doyle in 2015. Afterwards, he conducted postdoctoral research with Prof. Stefan Hecht at Humboldt-Universität zu Berlin until 2018, before returning to Taiwan for mandatory military service and industrial research at ScinoPharm Taiwan. He began his independent career at ICReDD as Associate Professor and Junior-PI in November 2021.



About ICReDD

The development of new chemical reactions is intrinsically entangled with the prosperity of humanity and the preservation of the environment. A recent example of such transformative chemical reactions with profound impact is cross-coupling reactions, the discovery of which was awarded with the 2010 Nobel Prize in Chemistry. These reactions are used to produce approximately 20% of all medicinal reagents, and almost all liquid crystalline and organic electroluminescent materials. The industrial use of these chemical reactions contributes ~60 trillion yen per annum to the global economy. The development of new chemical reactions thus significantly affects the evolution of society.

ICReDD is the Institute for Chemical Reaction Design and Discovery, a WPI center at Hokkaido University where researchers from different disciplines combine their strengths to take full control over chemical reactions. The institute was born out of the realization that the purposeful design of chemical reactions requires cross-sectional collaborations at every step. Working on such a fundamental natural process, quantum-chemical computations, information technology, modern experimental techniques, and the development of advanced materials can no longer be separate fields if we want to achieve significant breakthroughs. Rather, they have to become part of a diverse toolbox for truly integrated research.

The CATALYST is inspired by catalysts used in chemistry to bring molecules together, to reduce reaction barriers, and to activate molecules—to make reactions happen faster. In this spirit, this poster series should enable its readers to make the connection between chemical reactions and the wellbeing of our society, and to look at the world in a new way, seeing how chemical reactions and chemistry shape the world around them. And if we can take this opportunity to introduce ourselves, too, this may also catalyze new friendships and opportunities. #ReactWithUs

React With Us!

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with what's happening at ICReDD,
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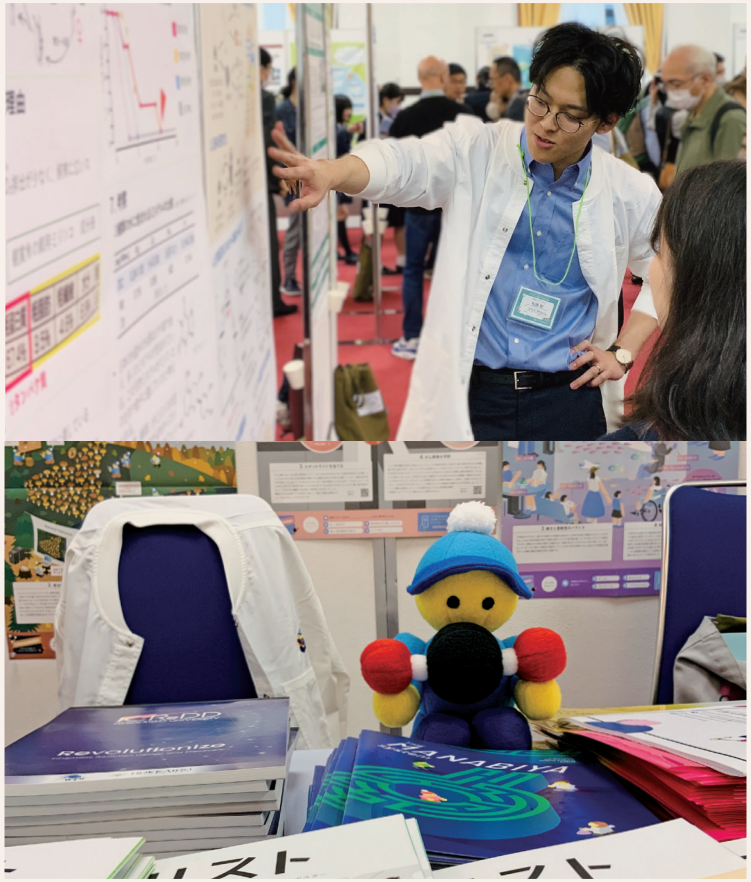

The 13th WPI Science Symposium was held at Kyoto University on November 16th (Sat.).The WPI Science Symposium aims to showcase the latest research at WPI and to introduce the fun of science to the general public, especially high school students.This year the event consisted of two parts: science talks by WPI researchers in the morning and poster presentations and discussions by high school students and WPI researchers in the afternoon.(Top) Assistant Professor Wataru Matsuoka of ICReDD gives a presentation of AFIR, a computational method for exploring chemical reaction pathways. (Bottom) All issues of CATALYSTs and ICReDD goods were distributed at the ICReDD booth.

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