The CATALYST

Helping you react with chemical reactions

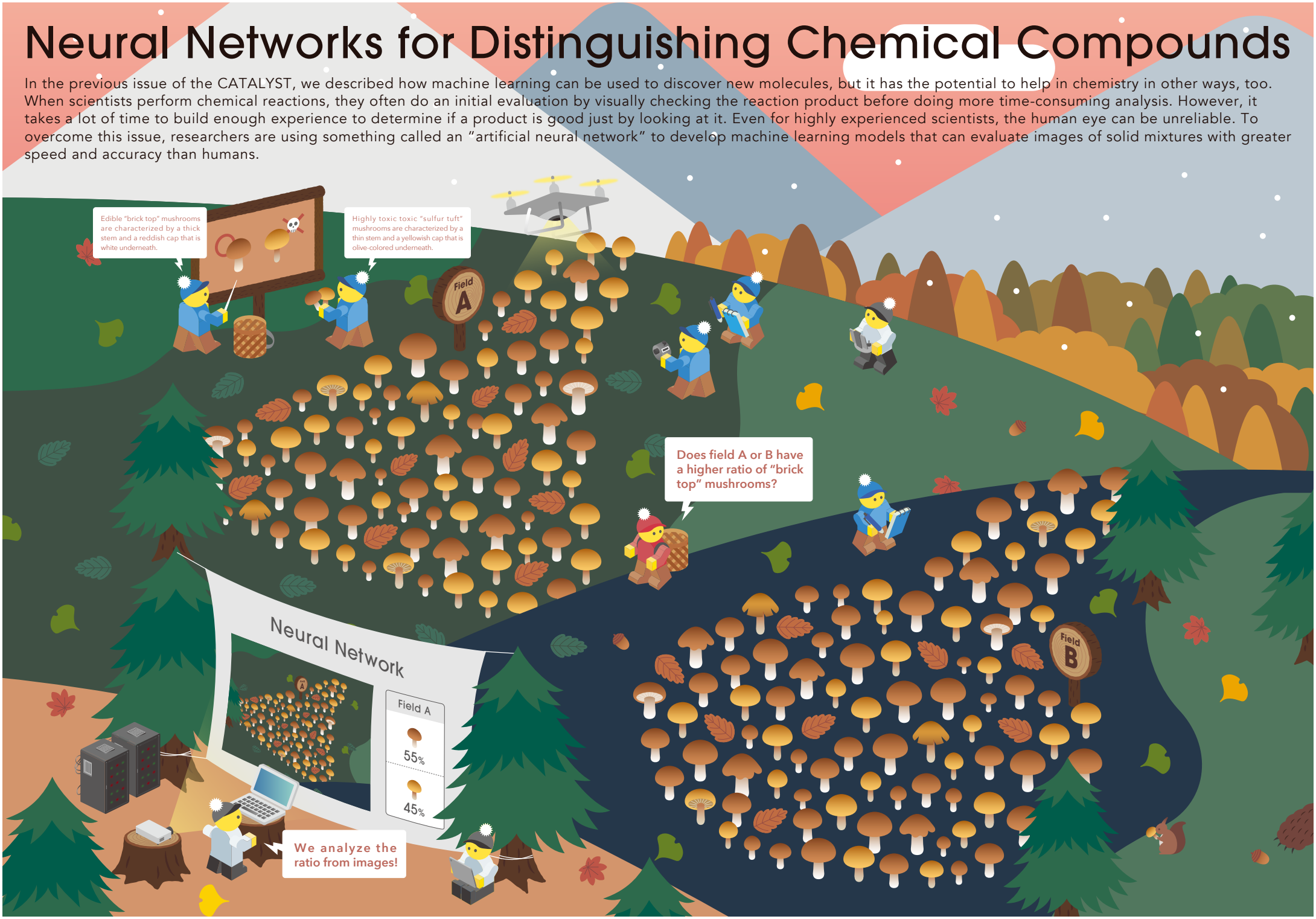
Issue 14
December 2023

Neural Networks for Distinguishing Chemical Compounds

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

Neural Networks for Distinguishing Chemical Compounds

In the previous issue of the CATALYST, we described how machine learning can be used to discover new molecules, but it has the potential to help in chemistry in other ways, too. When scientists perform chemical reactions, they often do an initial evaluation by visually checking the reaction product before doing more time-consuming analysis. However, it takes a lot of time to build enough experience to determine if a product is good just by looking at it. Even for highly experienced scientists, the human eye can be unreliable. To overcome this issue, researchers are using something called an "artificial neural network" to develop machine learning models that can evaluate images of solid mixtures with greater speed and accuracy than humans.

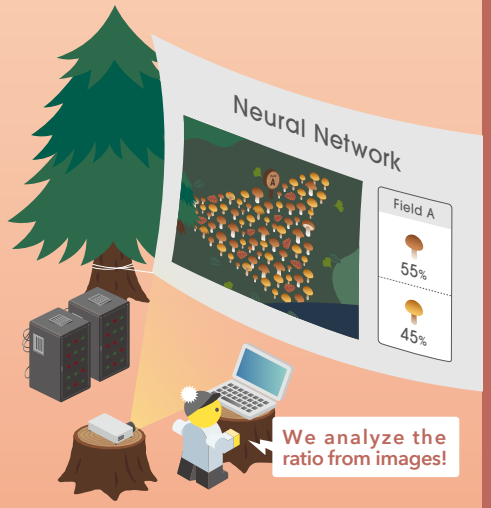


1. Humans distinguishing things

Have you ever accidentally ruined a recipe in the kitchen by adding salt instead of sugar? It's an easy mistake to make! Our brains tell different objects apart by identifying their distinguishing features. In the case of salt and sugar, they are both small crystals with a white color. Our brains have trouble distinguishing them because their features are quite similar to each other. Edible and poisonous mushrooms are another example of things that can have similar features and be hard to distinguish. Although difficult, if you aren't able to recognize the small differences in appearance, you can be in real trouble! When going to pick mushrooms in the mountains, firstly it is important to distinguish edible mushrooms from poisonous mushrooms, but if you could also know ahead of time which fields have the highest ratio of edible mushrooms, it would make picking safer and more efficient.

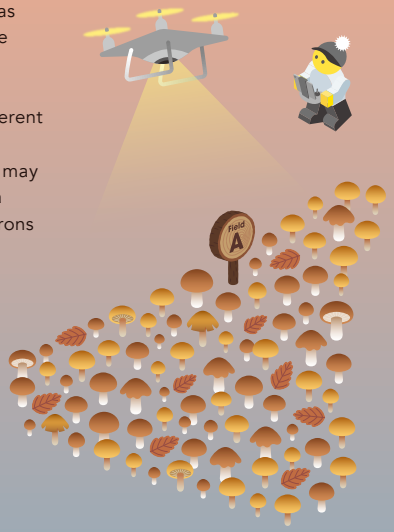
2. Computers distinguishing things

Computers can distinguish images using something called an artificial neural network, which mimics the way neurons (nerve cells) in our brain send and receive information via electrical signals. In artificial neural networks, artificial neurons, which can be thought of as switches, are organized into connected layers. The first layer receives the image, and each neuron analyzes a small part of the image. If that part of the image meets a specific condition, the neuron will switch "ON" and send information forward to the next layer. Otherwise it will stay "OFF". This process of layers receiving and sending signals repeats, with each subsequent layer analyzing increasingly complex features. When the signals reach the final layer, the neural network distinguishes the image based on those signals.



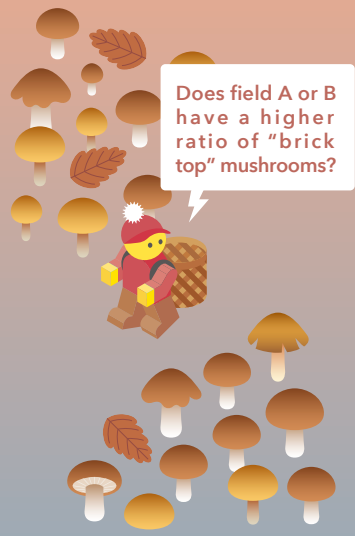
3. Identifying Features

Artificial neural networks show promise as tools that can recognize features that are difficult for even trained experts to distinguish. In chemistry, artificial neural networks can be used to distinguish different solid chemical compounds in images. Neurons in the first layer of the network may switch on when a basic feature such as a curve or a sharp point is identified. Neurons in the next layer could check for more detailed features comprised of basic features in a certain arrangement. By being trained on lots of example data, it is possible for the neural network to distinguish subtle differences in color, shape and size that are difficult to discern with the human eye and then use those characteristics to identify chemical compounds.



4. Evaluating solid mixtures

In addition to identifying product compounds from an image, artificial neural networks can also utilize information about the number of times that product appears in an image to determine the ratio of components in a mixture. Researchers at ICReDD created a neural network-based model that successfully identified the ratio of sugar and salt in a mixture of the two, and the model's accuracy was twice as high as the best performing member of the research team! Researchers further tested their model, demonstrating its ability to analyze 4-component mixtures of chemical compounds and to monitor the progress of product formation in a solid-state reaction. This technology could enable quicker, more accurate product confirmation in lab and be used in industry to efficiently monitor reactions performed in chemical plants.



Activation!

Quiz

What is the ratio of brick top mushrooms to sulfur tuft mushrooms in Field B?

Send us your answer!

- A: 70% / 30%
- B: 65% / 35%
- C: 60% / 40%
- D: 55% / 45%

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

December 2023

New Researchers

Narendra Nath Pati
Organic synthesis, porphyrin chemistry

Navpreet Kaur
Asymmetric catalysis

Vitor Alcantara Fernandes da Silva
Organocatalysis, asymmetric catalysis

Sagar Ghorai
Computational chemistry, polymers

Yongjie Shen
Computational catalysis, catalytic degradation

Selected Publications (from September 2023 to November 2023)

Surpassing the human eye: machine learning image analysis rapidly determines chemical mixture composition
(Y. Ide, S. Hu, I. Takigawa, Y. Inokuma)
https://www.icredd.hokudai.ac.jp/research/9856

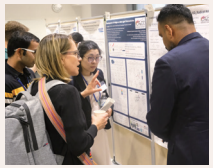
Making elbow room: Giant molecular rotors operate in solid crystal
(H. Ito, M. Jin)
https://www.icredd.hokudai.ac.jp/research/9935

ICReDD researchers summarize state-of-the-art in computer-guided development of reaction methodologies
(H. Hayashi, S. Maeda, T. Mita)
https://www.icredd.hokudai.ac.jp/research/10029

Development of machine learning framework for automatically extracting detailed synthesis procedures from organic chemistry articles
(S. Akiyama, Y. Nagata, M. Yoshioka)
https://www.icredd.hokudai.ac.jp/research/10123

Symposia

- The 6th ICReDD International Symposium and 3rd Akira Suzuki Awards Ceremony
- List Sustainable Digital Transformation Catalyst Collaboration Research Platform Kickoff Symposium
- The 12th World Premier International Research Center Initiative (WPI) Science Symposium



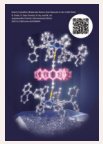
The 6th ICReDD International Symposium

List Sustainable Digital Transformation Catalyst Collaboration Research Platform Kickoff Symposium

Outreach

- Monthly Research Postcard
- The CATALYST Issue 13

The CATALYST 13th Issue



Monthly Research Postcard

Award

- 2024 Skolnik Award (Varnek)

Researcher Profile

vol.14

Yuki Ide

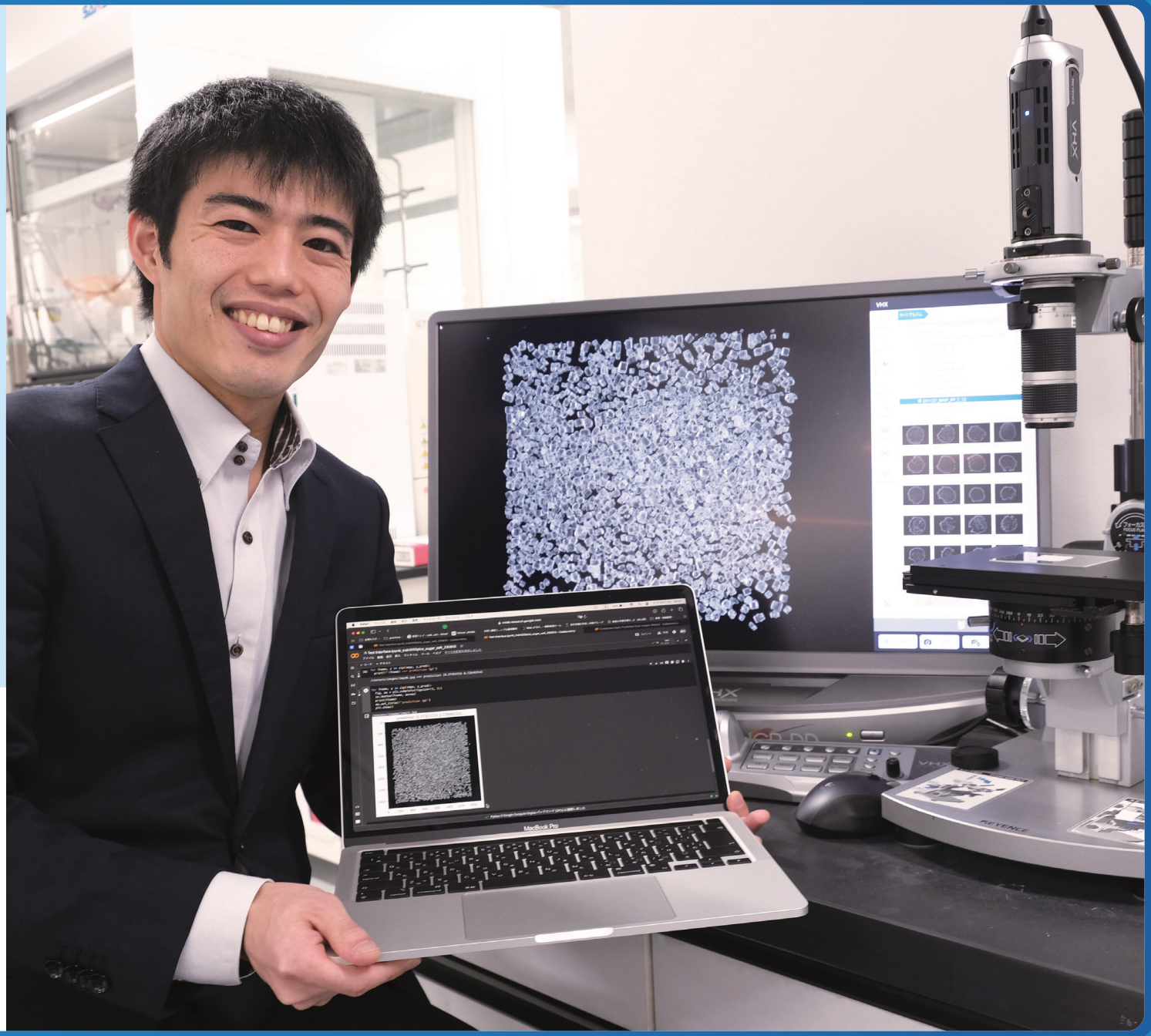
Specially Appointed Assistant Professor Ide aims to incorporate machine learning systems into chemistry research and extend that to real-world applications. In particular, he builds machine learning systems that can instantly analyze the mixing ratio of solid mixtures such as sugar and salt.

Representative Papers:

Ind. Eng. Chem. Res. 2023, 62, 13790-13798;
Chem. Sci. 2022, 13, 9848-9854;
Dalton Trans. 2017, 46, 242-249

Short Biography

ICReDD Specially Appointed Assistant Professor. In 2018, Professor Ide received his PhD from the Interdisciplinary Graduate School of Science and Engineering at Shimane University. From 2018, he was a program-specific researcher at the Institute for Chemical Research (ICR) in Kyoto University. In April 2020, he started his current position.



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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@ICReDDconnect

In November, ICReDD hosted The 12th World Premier International Research Center Initiative (WPI) Science Symposium, which aims to convey WPI research to non-scientists, with a focus on middle and high school students. (Top) After giving individual talks on using information science in fusion research, three researchers joined together on stage for a panel discussion. (Bottom) WPI research was showcased in various ways, including a hands-on VR experience, during a booth exhibition featuring all 18 WPI research institutes.

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