Research Strategy

ICReDD's fusion research creates a feedback loop that uses the results of basic and applied experimental science to improve the design and efficiency of computational and information science tools that accelerate and automate chemical reaction discovery.

Our research foundation

ICReDD uses the artificial force induced reaction (AFIR) method, a state-of-the-art reaction path search method based on quantum chemical calculations, and applies information science in order to extract meaningful information that can narrow down optimal experimental conditions. This approach pinpoints promising experiments, thus reducing time consuming trial and error in the lab.

Our innovative approach has led to advancements in the automation of reaction development:

Ligand/Catalyst Design:
Ligand screening is a laborious but critical step in the catalyst design process. ICReDD has developed a virtual-ligand assisted (VLA) screening method, which enables the rapid computational screening of a broad range of ligand properties to determine what ligand properties will give the highest selectivity for a reaction.

Reaction Design:
Until now, computer simulations have been primarily used by chemists to analyze the reaction pathways of reactions discovered in the lab. However, researchers at ICReDD have taken a major step forward and used simulations based on the AFIR method to produce the general idea for an entirely unimagined reaction, synthesizing 48 different compounds based on the predicted reaction type.

Reverse reaction prediction:
Predicting the recipe for a target product molecule, with no knowledge other than the target molecule itself, would be a powerful tool for accelerating the discovery of new reactions. Our researchers have developed an algorithm to handle more complicated systems and can now use AFIR to perform reverse reaction prediction of multi-step reactions.

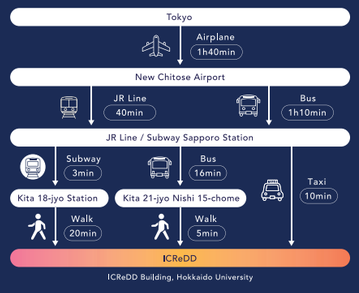
Principal Investigators

Support ICReDD

-**Support** overseas research travel and development of young researchers
-**Support** start-up projects and fusion research initiated by young researchers
-**Support** the organization of public lectures and outreach activities
-**Support** the acquisition of new equipment and hiring of research support staff

"Humans have utilized a wide range of chemical reactions to improve the quality of our everyday life. Our research at ICReDD seeks to increase the frequency at which life-changing chemical reactions are discovered. We hope you will support ICReDD's efforts towards creating a prosperous future society through research."

G. Maeda



ICReDD

Social media: @ICReDDconnect

About WPI

The World Premier International Research Center Initiative (WPI) was launched in 2007 by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) in a push to build within Japan globally visible research centers that boast a research standard and research environment outstanding enough to prompt top tier researchers from around the world to want to work in them. ICReDD was established in October 2018 at Hokkaido University.

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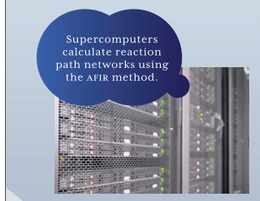
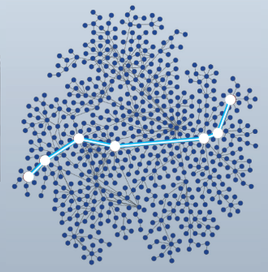
ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

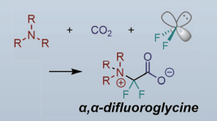
Revolutionizing
chemical reaction design
and discovery

ICReDD's vision for fusion research



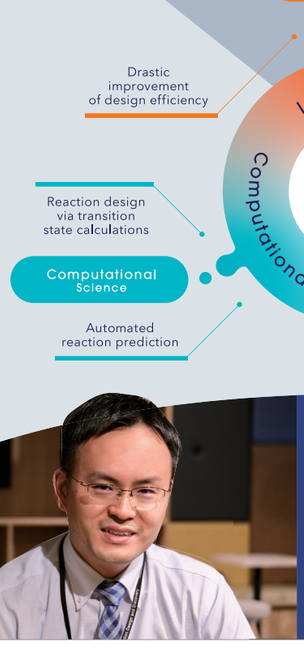
Supercomputers calculate reaction path networks using the AFIR method.





Information scientists process massive data and identify promising paths.

Experimental scientists verify these paths. Less trial and error accelerates new reaction discovery!



Message from Satoshi Maeda, Director of ICReDD

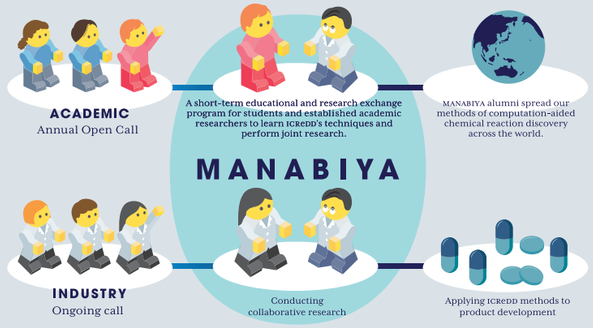
Reaction development that relies solely on the trial-and-error approach is too time-consuming to solve urgent global problems, including pollution as well as energy and resource scarcity.

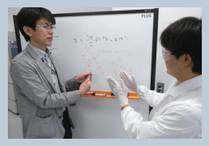
ICReDD is revolutionizing the traditional approach to developing reactions by fusing computational, information and experimental sciences. We strive to spread the benefits of this approach by integrating other disciplines to explore novel applications. It is our sincere hope that our institute may contribute to a brighter and more prosperous future for all of humanity.

Features of the Institute

MANABIYA System

A short-term educational and research exchange program





Establishing a New Graduate School

ICReDD plans to expand the MANABIYA system into a full-fledged graduate program, creating the graduate school of "*Chemical Reaction Design and Discovery*" in Hokkaido University. This graduate school will bring fresh ideas to graduate education at Hokkaido University and create next-generation graduates who are proficient in all three disciplines: experimental, computational and information science.

Industrial Collaboration (Mitsui Chemical)

In 2023, ICReDD and Mitsui Chemicals launched a 5-year, large-scale joint research initiative, including a joint laboratory housed in the ICReDD building. ICReDD places a strong importance on turning our chemical reactions into benefits for society.

List Research Platform

The List Sustainable Digital Transformation (DX) Catalyst Collaboration Research Platform, led by 2021 Nobel Laureate in Chemistry Benjamin List, was established within ICReDD in 2023. This platform utilizes techniques developed at ICReDD to create novel, efficient methods for designing new organocatalysts.

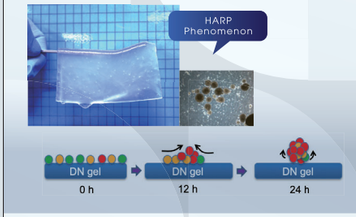
ICReDD Fellows

ICReDD adopts a flexible personnel structure with regularly rotating PIs. ICReDD Fellows are researchers inside and outside of Hokkaido University who are given access to ICReDD's resources to perform joint research and this group of fellows are potential candidates to be future ICReDD PIs.

New Technologies

New Tools for Cancer Drug Development

Cancer specialist Professor Tanaka collaborated with hydrogel specialist Professor Gong to discover that culturing differentiated cancer cells in a double-network hydrogel causes them to revert into cancer stems cells. This provides a way to easily test prototype drugs that target these stem cells and could potentially reduce cancer recurrence.

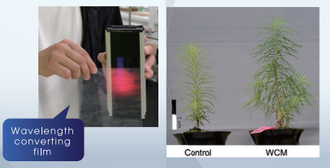


Selective Catalyst Prediction

Professor Tsuji of the List Group collaborated with Professor Sidorov and Professor Nagata to develop a semi-automated system for predicting highly selective catalysts without using expensive quantum chemical calculations. Using a synthesis robot, they produced experimental data for training a machine learning model that was then able to predict new catalysts of higher selectivity than those used in the training data.

Acceleration of Plant Growth

Professor Hasegawa's group has developed luminescent europium-based materials with a wide variety of applications. A collaboration with the Hokkaido University Research Faculty of Agriculture found that europium-based thin films that convert UV light to red light could be used in greenhouses to accelerate plant growth through the promotion of photosynthesis.



Solid-state, mechanochemical reactions

In mechanochemical reactions, solid reactants are put inside a small jar with a ball and then shaken, causing them to react despite the use of little to no solvent. Professor Ito's group used this method to perform new reactions with poorly soluble reactants and developed cost effective, simple, and environmentally friendly ways of performing important reactions including the Birch Reduction and the synthesis of Grignard reagents.