



The CATALYST

Helping you react with chemical reactions

Issue
5

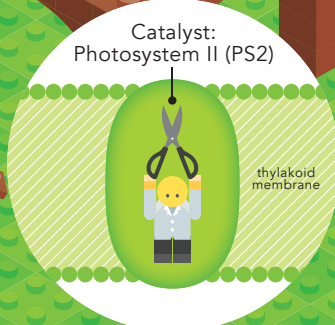
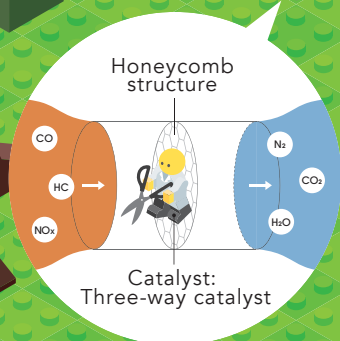
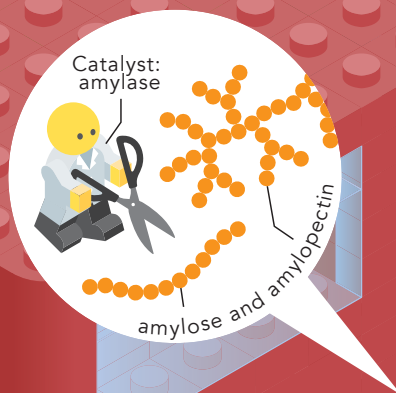
September
2021

How Catalysts Work

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

How Catalysts Work

At ICRéDD, we are studying how to develop new chemical reactions efficiently and rapidly. One method is the study of catalytic reactions. A catalyst is a substance that acts as a "medium" for a chemical reaction. Catalysts interact with the reacting chemicals to change the rate of the reaction, but do not undergo a permanent change themselves. Let's get to know the catalysts around us and learn about the catalysts we are studying at ICRéDD.



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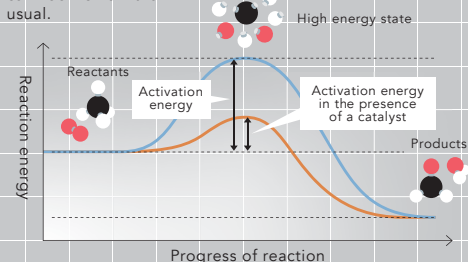
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How catalysts work

We learned in the first issue that in order to break a bond between atoms of a molecule and combine it with another atom in a chemical reaction, a specific bond in the molecule must be broken and pass through a state of high energy. The energy required to get to this state is called activation energy. When a catalyst is used, this activation energy is lowered, making it easier for the reaction to proceed.

Relationship between catalyst and reaction energy

By using a catalyst, the activation energy can be lower than usual.



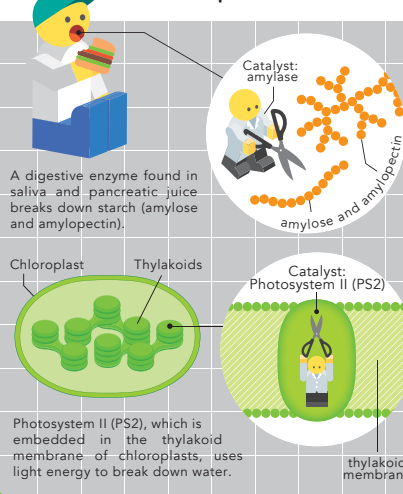
Level

2

Naturally occurring catalysts

In the body, the action of digestive enzymes breaks down carbohydrates into glucose, proteins into amino acids, and fats into fatty acids, etc. The enzymes do not change before or after the decomposition reaction, but only facilitate the reaction. Photosynthesis uses the sun's energy to produce carbohydrates and oxygen from carbon dioxide and water. Photosynthesis is not a single reaction, but consists of many reactions. It includes a catalytic reaction that uses light energy to break down water.

Catalysts in the human body and in plants



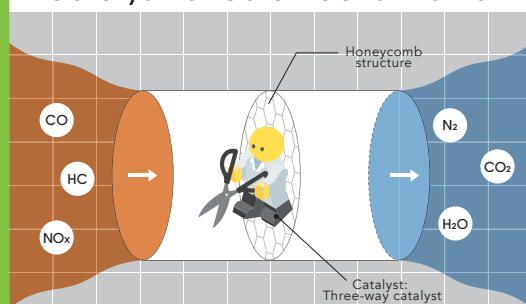
Level

3

Catalysts incorporated into automobile mufflers

Precious metals such as platinum, rhodium, and palladium are artificial catalysts used in industrial products. Three-way catalysts are used to purify exhaust gases from automobiles and other vehicles through catalytic reactions. Other catalysts are also used to make many chemical products from petroleum and other materials.

Catalyst for automobile muffler



Three-way catalysts in car mufflers are coated with platinum, rhodium, and palladium on the surface of honeycomb-shaped ceramics to purify carbon monoxide, hydrocarbons, and nitrogen oxides in exhaust gas.

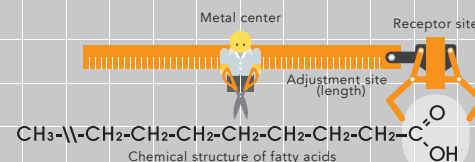
Level

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Research at ICRReDD

In ICRReDD, we have modeled chemical reactions using the most advanced chemical reaction simulation methods in the world. As a result, we have developed a groundbreaking artificial catalyst that can efficiently synthesize various useful organic compounds from fatty acids. This is important because fatty acids are a chemical raw material of biological origin (biomass) that provide an alternative to petroleum. The production of biomass through photosynthesis consumes carbon dioxide, thus it is expected that transitioning from the use of petroleum-derived raw materials to biomass will contribute to the realization of a sustainable society.

Catalysts developed by ICRReDD



Our new catalyst has an adjustable site by which the length of the catalyst can be changed. By changing this length, it is possible to select a specific carbon-hydrogen bond to undergo the reaction, producing different organoboron compounds. These compounds can then be further converted into various forms.

Activation

Quiz

A catalyst itself does not change, but makes it easier for a reaction to proceed by lowering the ____.

Send us your answer!

- 1) Activation energy
- 2) Pressure
- 3) Sun's energy
- 4) Humidity

Challenge

Send us if you find any catalysts around you.

Share your answer on social media!

#ReactWithUs
@ICReDDconnect

NEWS

New Researchers



Gwee Shu
Hui Eunice

Mathematical
modelling of plant
hormone flow



Ruben Staub

Machine Learning for
Chemistry, Active
Learning



Clement Fang
Jin Koh

Polymer Networks
and Gels

Selected Publications

(from May 2021 to July 2021)



Development of a Simple
Method for Preparing
Luminescent Polymers

(K. Kubota, S. Maeda, M. Jin, H. Ito)

DOI: [10.1002/anie.202105381](https://doi.org/10.1002/anie.202105381)

Computationally Designed
Synthesis of Difluoroglycine
Derivatives from Amines,
Difluorocarbene, and Carbon
Dioxide

(H. Hayashi, H. Takano, H. Katsuyama,
Y. Harabuchi, S. Maeda, T. Mita)

DOI: [10.1002/chem.202100812](https://doi.org/10.1002/chem.202100812)

Single-molecule
nanospectroscopy

(T. Iwasa, T. Taketsugu)

DOI: [10.1126/science.abg8790](https://doi.org/10.1126/science.abg8790)

A fluorescent metal-ion
detector generated from a
'masked' tetraketone

(Y. Kitagawa, Y. Hasegawa, T. Yoneda,
Y. Ide, Y. Inokuma)

DOI: [10.1002/ejoc.202100784](https://doi.org/10.1002/ejoc.202100784)

Unlocking the Mysteries
Behind the Synthesis of the
"Pigments of Life"

(Y. Ide, J. Pirillo, Y. Hijikata, T. Yoneda,
Y. Inokuma)

DOI: [10.1021/jacs.1c06331](https://doi.org/10.1021/jacs.1c06331)

Symposia (invited and more)

- WPI Online Seminar for Educators: ICRDD x I²CNER "Relatable State-of-the-Art Chemistry" (T. Nakajima)
- RIKEN AIP Open Seminar (I. Takigawa)
- Symposium for Reaction Path Search 2021 (T. Komatsuzaki, K. Suzuki, T. Mita)

〈Co-organized Symposium〉

- The 33rd Banyu Sapporo Symposium
- The 15th Annual Meeting of Japan Society for Molecular Science 2021

Awards

- Japanese Association for Molecular Target Therapy of Cancer Excellent Presentation Award (M. Tsuda)

Outreach

- Monthly news postcards
- Quarterly news poster
The CATALYST 4th issue

React With Us!

To stay up to date
with what's happening at ICRDD,
follow us on our social media channels:

@ICReDDconnect



Research Facilities

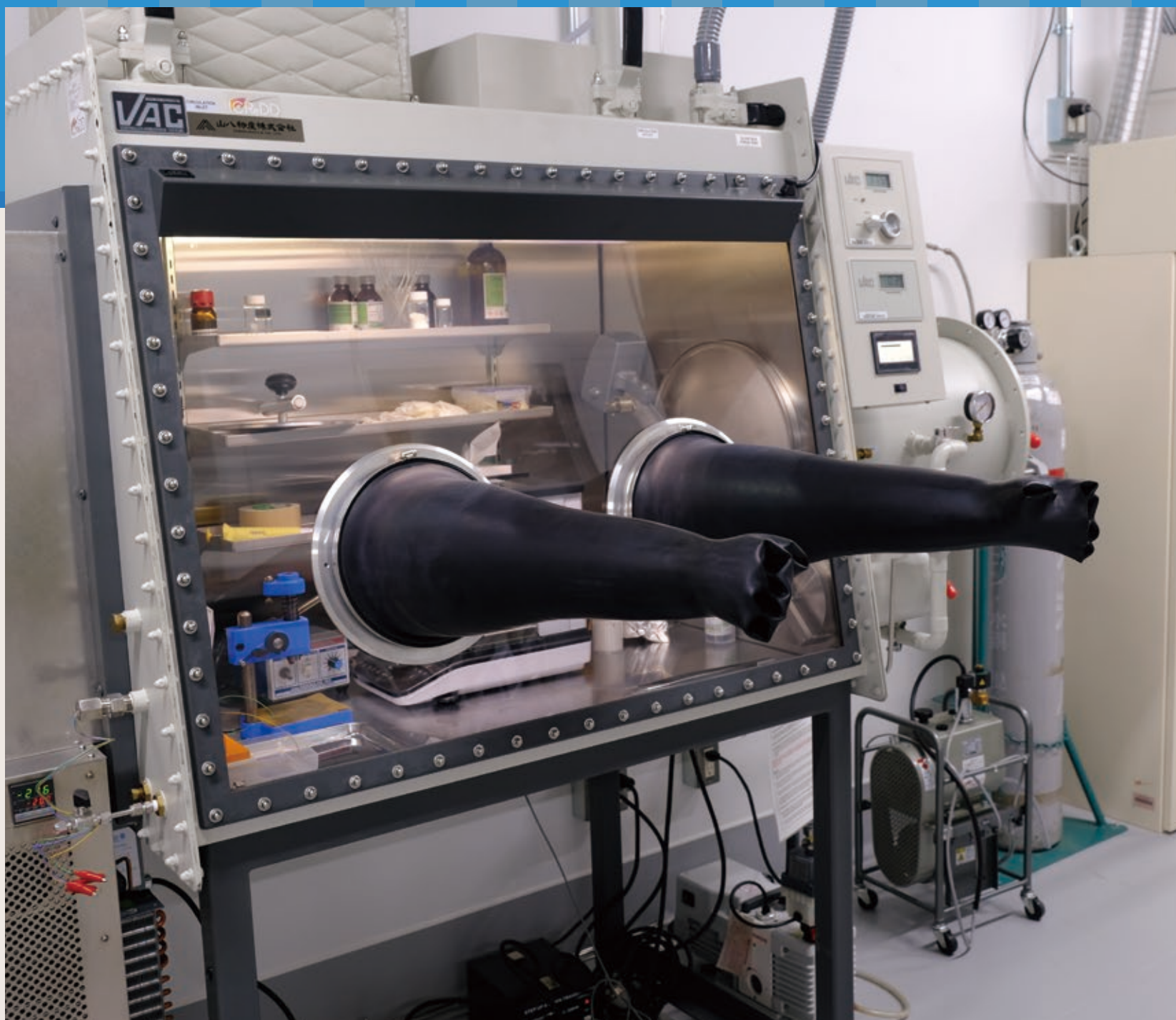
Glovebox

The black glove protruding outward has the fingertips folded inward. The fingertips are aligned here and the hand is inserted into the box to perform the experiment. Catalytic reaction development also begins in this glove box.



Overview

Glove boxes are used to safely handle metal complexes (catalysts) and compounds that change or decompose when exposed to oxygen or moisture. Glove boxes are equipped with a device to remove oxygen and moisture to prevent them from being affected by oxygen and moisture, and are used to work in an environment where inert gases such as high-purity nitrogen and argon filled inside are circulated to keep the atmosphere at a constant level, almost free of oxygen and moisture.

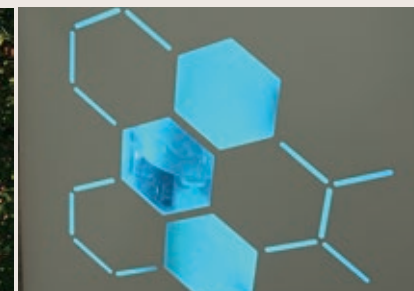


About ICReDD

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



Photographed before the pandemic

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