



The CATALYST

Helping you react with chemical reactions

Issue

3

March
2021

Propose
the optimal
chemical reaction!

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

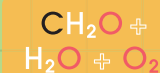
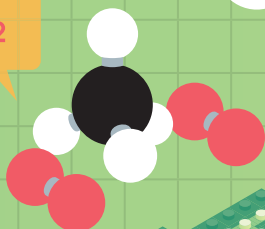
Propose the optimal chemical reaction!

The use of technologies such as telework, online classes, online events, telemedicine, IoT, 5G, big data, VR, etc. are becoming more and more common.

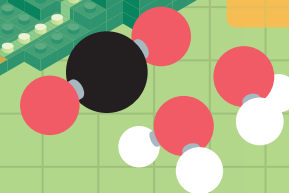
At ICReDD, we are studying how to efficiently and rapidly develop new chemical reactions that will be necessary for society in the future by integrating computational science, information science, and experimental science. Let's learn how to develop chemical reactions rapidly using information science.



START



GOAL

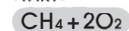


optimal route

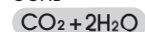
Search results

1

START:



GOAL:



ENERGY



START

GOAL



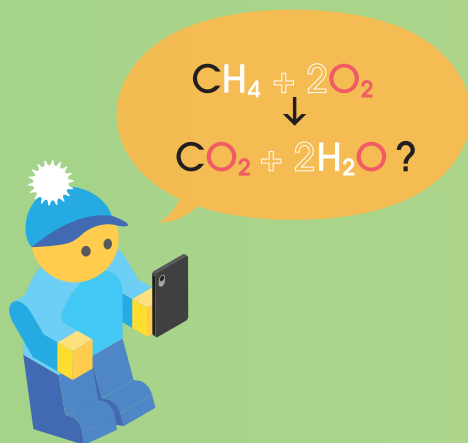
Here is the feasible optimal route. There is one other route that can be rearranged to one molecule of formaldehyde, one molecule of water, and one molecule of oxygen.

Level

1

What is Society 5.0?

Society 5.0 is a society in which virtual space and real space are highly integrated. Specifically, Society 5.0 is a society that follows Society 1.0 (hunting society), Society 2.0 (agricultural society), Society 3.0 (industrial society), and Society 4.0 (information society).



Level

3

The future society that Society 5.0 aims to create

Society 5.0 will solve these issues of the information society by utilizing technologies such as artificial intelligence (AI) and robotics. Image processing, machine learning and other technologies will make it possible to speed up search technology, advancement of search technology for car navigation systems, introduction of automated driving technology into cars and buses and its use in agriculture, construction, and disaster sites, go cashless, advance translation technology, automate factories with robots, and use drones for agriculture and delivery. Everything will be possible.

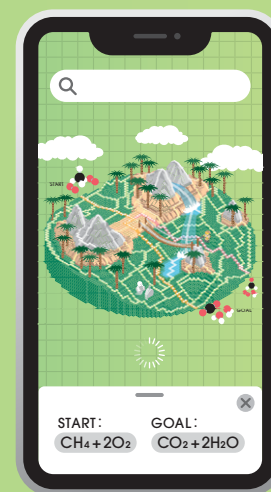


Level

2

The issues of Society 4.0

In Society 4.0 (Information Society), with the development of computers and the Internet, the IoT is advancing and all the things around us are connected to the Internet, collecting a lot of data and information, and handling a huge amount of information. As a result, it is difficult to find the information you want when searching for information, and even when using a car navigation system, there are many routes to the destination, and traffic jam information must be taken into consideration.

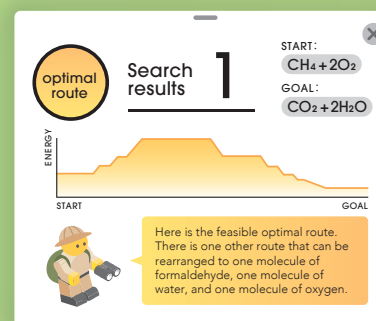


Level

4

ICReDD's technology for proposing optimal chemical reactions

At ICReDD, we use computational science to estimate the energy required for chemical reactions, and design and develop new chemical reaction mechanisms. However, the data estimated by calculation has vast information quantity and it is similar to a route search of a car navigation system. With the use of information science such as AI, it will be possible to quickly propose feasible reactions from a vast amount of chemical reaction paths data.



Activation

Quiz

Society 5.0 is a society in which _____ space and real space are highly integrated.

Send us your answer!

- 1) two-dimensional
- 2) three-dimensional
- 3) inter-dimensional
- 4) virtual

Challenge

Find Society 5.0 on a daily life.

Send us your answer!

Share your answer on social media!

#ReactWithUs
@ICReDDconnect

NEWS

New Researchers



Satoru Iwata

Optimization methods in computational chemistry and chemoinformatics



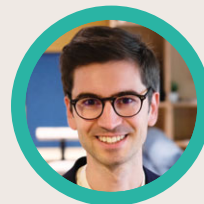
Xihong Wang

Organometallic chemistry, design new chiral ligands and new chemical reactions



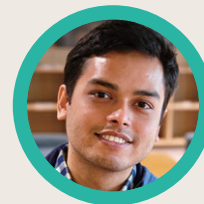
Sunao Shoji

Development of photofunctional lanthanide supramolecules based on computational quantum chemistry



Jean-Emmanuel Clement

Development of analytical frameworks by bridging Raman hyperspectral images and artificial intelligence



Ranajit Saha

Retention or retraction of chiral memory in polymers



Ravindra Krushnaji Raut

Development of organocatalytic reaction



Yong You

Development of new reactions, constructing new and interesting organic compounds

Symposia (invited and more)

- WPI Online Symposium 2020 for High School Students (N. Tsuji)
- Kanazawa University Sakigake Project 2020 Seminar 2nd Ohmiya Lab and Takeda Virtual Symposium (M. Sawamura)
- Joint Symposium of School of Science & WPI-ICReDD in Hokkaido University (C. Ozen, P. Sidrov, R. L. Reyes, H. Hayashi)
- 126th MSL Lecture in Tokyo Institute of Technology (Y. Inokuma)
- IQCE Quantum Chemistry Exploration Lecture 2020 (S. Maeda, T. Iwasa)
- Research Society in Institute for Molecular Science (T. Iwasa)
- New Horizons in Scientific Software (NHISS 2020) (T. Taketsugu)
- Joint Workshop of Research Center for Computational Science and Nanotechnology Platform Project (M. Kobayashi)
- 2020 the 5th lecture in Artificial Intelligence Advanced Research Center, Gifu University (M. Kobayashi)
- Dalian University of Technology-Overseas Partner Universities Series Online Exchange Conference (Y. Shimizu)

Awards

- Central Glass Company Award in the Society of Synthetic Organic Chemistry, Japan (H. Hayashi)
- Thieme Chemistry Journals Award (Y. Nagata)
- Hokkaido Science and Technology Incentive Award (T. Mita)

Outreach

- Monthly news postcards
- Quarterly news poster The CATALYST 2nd issue

Selected Publications

(out of 23 papers from November 2020 to January 2021)

Real-Time Probing of an Atmospheric Photochemical Reaction by Ultrafast Extreme Ultraviolet Pulses: Nitrous Acid Release from *o*-Nitrophenol
(T. Taketsugu)

DOI: [10.1021/acs.jpcclett.0c03297](https://doi.org/10.1021/acs.jpcclett.0c03297)



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Researcher Profile

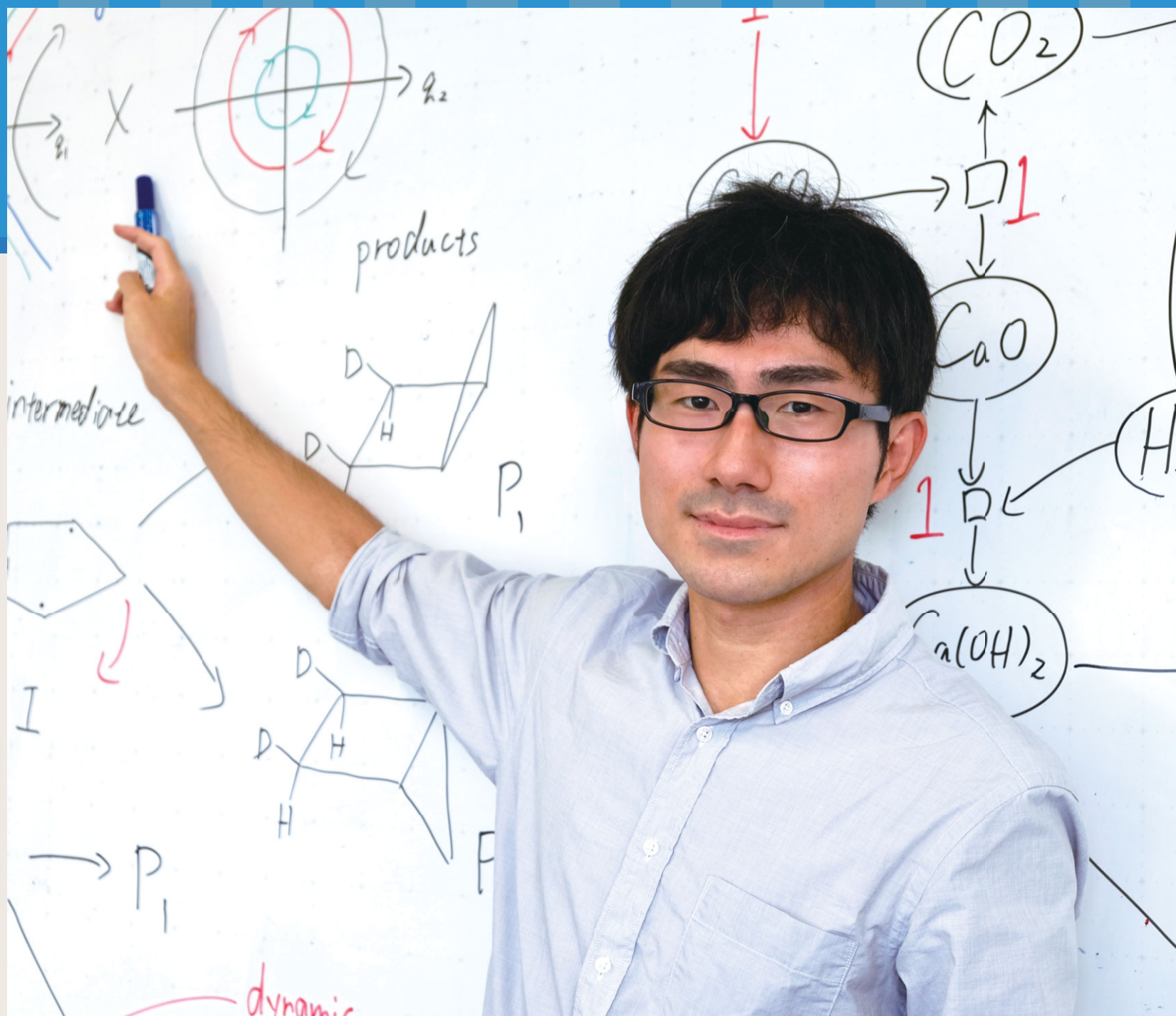
Yuta Mizuno

Yuta Mizuno studies information processing techniques for deciphering huge and complex networks of chemical reactions using quantum computers, future computers that utilize the physical laws of the microscopic world.

Short biography

Assistant Professor, Institute for Chemical Reaction Design and Discovery (WPI-ICReDD) concurrent with Research Center of Mathematics for Social Creativity, Research Institute for Electronic Science, Hokkaido University
Ph. D. from the University of Tokyo Graduate School of Arts and Sciences in 2018. Current position since 2019. Japan Science and Technology Agency PRESTO Researcher in the "Quantum Software" area since 2020.

He specializes in chemical reaction dynamics, chemical reaction network, phase space geometry, and quantum computing technology.



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



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