

## The CATALYST

Helping you react with chemical reactions





## **Chemical Reactions Are Everywhere**

At ICReDD, we conduct research on how to efficiently and quickly develop new chemical reactions. As we explained in the first issue, if we could calculate the energy level of every electron rearrangement, we should be able to estimate exactly where and how much energy would be needed. This would enable us to create everything and therefore make a huge contribution to society. Chemical reactions may sound like something special that happens only in the laboratory, but in fact, they are everywhere. In this issue, let's learn about the chemical reactions that we are all familiar with, and chemical reaction research at ICReDD! Level

#### Chemical Reactions Associated with the Activities of Plants and Animals

Chemical reactions occur every day in the bodies of living things and in the process of plant growth without us noticing it. For example, when animals digest food, enzymes (catalysts) break down starch into glucose, protein into amino acids, and fat into fatty acids. It also converts the nutrients produced by the digestion such as glucose and fatty acids into energy using the oxygen obtained from breathing, and release carbon dioxide. Plants use photosynthesis to convert light energy, water and carbon dioxide into carbohydrates (sugars and starches) and oxygen. Converting one substance into another, such as "breaking down" or "digesting," is all a chemical reaction.



## Level

Products around Us

We are surrounded by materials that enrich our lives, including iron (iron refining), plastics, water absorbents for diapers, OLEDs, liquid crystals, synthetic fibers, medicines, inks and dyes, and cosmetics. Many of these are produced from natural resources such as oil and minerals, using chemical reactions.

### Chemical Reactions Used in

iquid Cryston

pen ink

### Chemical Reactions

around Us

Level

Level

In addition to inside of the body of animals/humans and the growth of plants, chemical reactions are all around us. For example, when we bake bread, first of all, the yeast breaks down the sugar by fermentation to produce carbon dioxide and alcohol. Next, when the fermented dough is baked, the sugars and amino acids combine to form a fragrant substance. A nicely browned steak or grilled fish is also caused by the same chemical reaction. In addition, chemical reactions occurring invisible to human eyes, such as batteries (substances react chemically with each other inside the battery and release electricity), bleaching, and superglues, are also all around us.

Research at ICReDD

ICReDD designs and develops new mechanisms of chemical reactions by estimating the energy required for chemical reactions through computation. We are trying to design new chemical reactions that are useful and valuable to society, and to develop new materials from resources such as carbon dioxide, which until recently has been almost unusable. We are also expanding our understanding of the human body and other complex objects, and using chemical reactions to develop new analytical techniques and diagnostics for diseases.



# Activation



For a process to be defined as a chemical reaction, \_\_\_\_\_ must be produced. Send us your answer!

1) a new substance 2) the same substance 3) light 4) more mass

#### Challenge

Find one chemical reaction that is happening in your home on a daily basis. Send us a picture or video!



#ReactWithUs @ICReDDconnect

#### Anniversary

ICReDD Foundation Day - Established on October 23, 2018

#### Selected Publications

(out of 45 papers from July to October)

Borylation of Aliphatic Amides

Asymmetric Remote C-H

and Esters with a Modular

(M. Sawamura, R. L. Reyes, K. Suzuki,

DOI: 10.1126/science.abc8320

Iridium Catalyst

S. Maeda)

Kinetic Prediction of Reverse Intersystem Crossing in Organic Donor–acceptor Molecules (Y. Harabuchi, S. Maeda)

DOI: <u>10.1038/s41467-020-17777-2</u>

Hydrogels as Dynamic Memory with Forgetting Ability (K. Cui, J. P. Gong)

DOI: <u>10.1073/pnas.2006842117</u>

#### Symposia (invited and more)

Chiral Lanthanide

Device

Y. Hasegawa)

Lumino-glass for a Circularly

(Y. Kitagawa, M. D. J. Islam, S. Maeda,

DOI: 10.1038/s42004-020-00366-1

Polarized Light Security

- The 6th Hokkaido University Cross-departmental Symposium (Oral presentation: T. Mita, Y. Inokuma, Poster presentation: Y. Nagata, T. Yamamoto)
- 10th CSJ Chemistry Festa (I. Takigawa)
- Symposium SRPS2020 (T. Taketsugu)

NEWS

Understanding the Interac-

tions between the Bis(trifluo-

romethylsulfonyl)imide Anion

X-ray Diffraction Analysis of a

Soft Crystal Surrogate (Y. Hijikata,

and Absorbed CO<sub>2</sub> Using

DOI: 10.1038/s42004-020-00390-1

J. Pirillo)

- The 6th Quantum Science (QS) Symposium (ICCMSE 2020) (T. Taketsugu)
- Minisymposium on Polymer Nanocomposites (M. Rubinstein)
- Establishing International Research Network of Mathematical Oncology Fusion of Mathematics and Biology (M. Imajo)

#### Summer Course

 Hokkaido Summer Institute (Online, August 24-26)
Advanced Computational Chemistry (K. Suzuki, A. Lyalin, M. Rubinstein, A. Varnek, I. Takigawa)

#### Outreach

- Monthly news postcards
- Quarterly news poster The CATALYST 1st issue
- Annual report 2019-2020

#### **TV** Coverage

• NHK News program "Ohayo Hokkaido" (Sawamura group, August 21)

#### React With Us!

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

#### @ICReDDconnect





Researcher Profile



ICReDD researcher Cihan Özen wants to decipher the mechanism of chemical reactions. Much of that is inaccessible by experiments, so he uses supercomputers to model the reactions.

#### Short biography

Postdoctoral Fellow at ICReDD After his Ph.D. in Chemistry from Istanbul Technical University in Turkey, Project Officer at BASF, Research Assistant at TÜBİTAK, and Lecturer at Piri Reis University respectively. In 2016, a visiting scholar at University of Miami via the Fulbright Visiting Scholar Program. Subsequently current position since April 2019. He specializes in reaction mechanism, homogeneous catalysis, and DFT (Density Functional Theory).



#### 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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