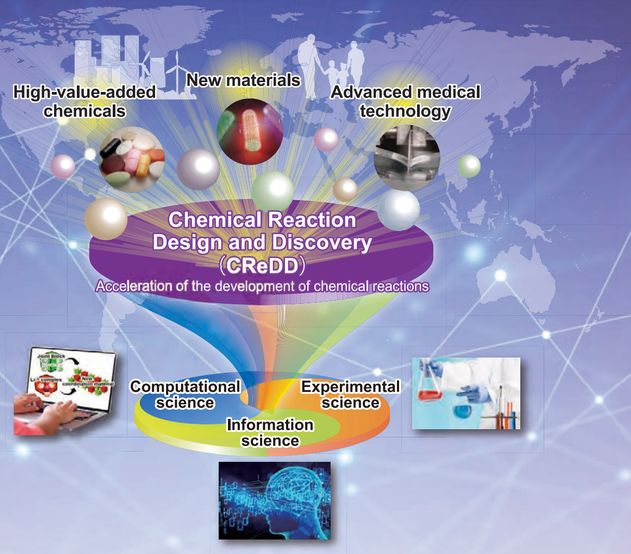
Introduction of the Institute for Chemical Reaction Design and Discovery (ICReDD)

In-depth understanding and efficient development of chemical reactions through the interdisciplinary research of computational science, information science, and experimental science.



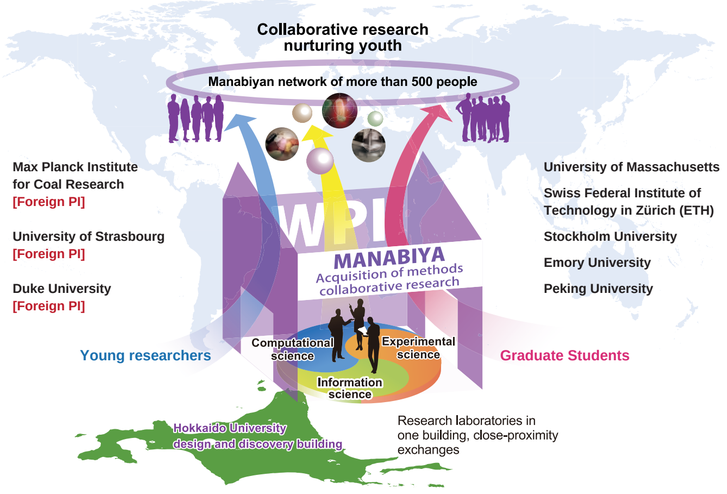
Message from Satoshi Maeda, Director of ICReDD

Reaction development that relies solely on the trial-and-error approach is too time-consuming to solve current global problems that include pollution as well as the scarcity of energy and resources.
“CReDD” will revolutionize the traditional approach to developing reactions by fusing computational, information, and experimental sciences. We strive to spread the benefits of this approach by establishing a global WPI and integrating other disciplines. Our sincere hope is that our WPI may contribute to a brighter and more prosperous future for all of humanity.

Director Satoshi Maeda

Features of the Institute

The establishment of the CReDD, and the collaborations at MANABIYA



1 To establish the new academic field “CReDD” that integrates computational, information and experimental sciences in order to accelerate the efficiency of the development of new chemical reactions which is indispensable for a prosperous and sustainable future of humanity.

2 To establish the MANABIYA system to educate young researchers and graduate students in order to realize a global circulation system for world-class scientists in the integrative research area “CReDD” .

MANABIYA system:

Young researchers and students from domestic and overseas collaboration institutes stay at the ICReDD for about three months, mastering the new reaction development method through collaborative research, and each researcher will utilize it in the future. After 10 years, the MANABIYA network will comprise several hundreds of researchers, which will support the further development of this new field.

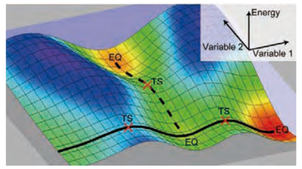
3 To implement organizational reform of the university centering on the establishment of the new graduate school “CReDD” .

Principal Investigators

Computational science

MAEDA, Satoshi [Director]

Mapping the reaction paths with the AFIR method

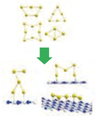


RUBINSTEIN, Michael

Theoretical calculation of polymer materials and macromolecules

TAKETSUGU, Tetsuya

Calculation of excited state species and design of heterogeneous catalysts



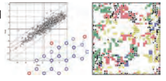
Information science

ARIMURA, Hiroki

Listing, selection, and high-speed search of small to medium-size molecules

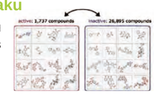
VARNEK, Alexandre

Reaction databases and molecular screening



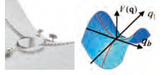
TAKIGAWA, Ichigaku

Reaction network modeling and data-driven predictions



KOMATSUZAKI, Tamiki

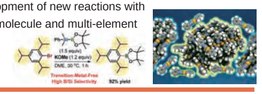
Mathematical modeling of macromolecule systems and data-driven science



Experimental science

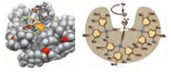
ITO, Hajime [Vice Director]

Development of new reactions with small molecule and multi-element



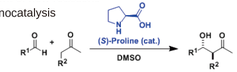
SAWAMURA, Masaya

Development of new catalytic reactions using transition metals



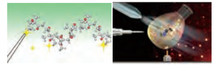
LIST, Benjamin

Development of new reactions using organocatalysis



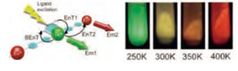
INOKUMA, Yasuhide

Small to medium-size molecule synthesis and crystallography



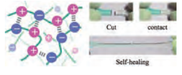
HASEGAWA, Yasuchika

Light-emitting materials with high brightness and durability



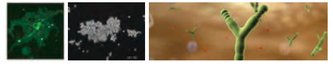
GONG, Jian Ping

Synthesis of biocompatible/self-evolving gels and macromolecules



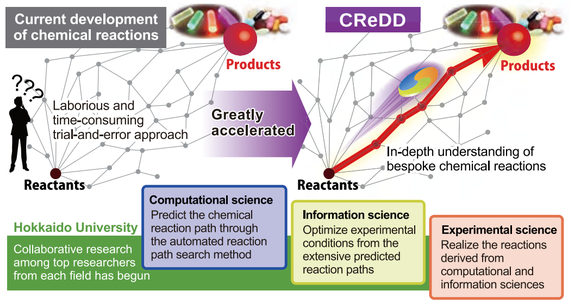
TANAKA, Shinya

Cell control by new materials, development of new generation diagnosis



Purpose of the Research

To realize high-level design and rapid development of chemical reactions



The current trial-and-error approach to the development of new chemical reactions is time-consuming and inefficient. The ICReDD uses state-of-the-art reaction path search methods based on quantum chemical calculations* and applies concepts of information science in order to extract meaningful information for experiments, thus narrowing down optimal experimental conditions. This approach enables “pinpointing” promising experiments.

The AFIR method
(Artificial Force Induced Reaction method)

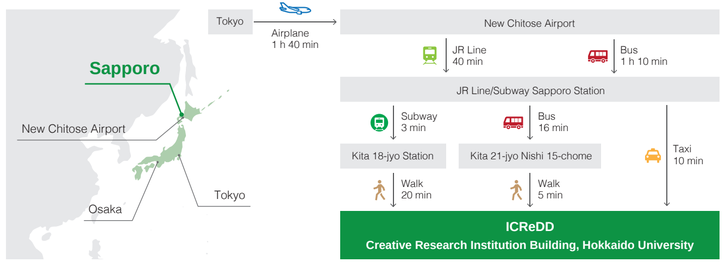
The only way to map the complicated reactions paths

Developed by Director: S. Maeda

*Maeda, S.; Morokuma, K. *J. Chem. Phys.* 2010, **132**, 241102.

In addition, data obtained by the experimental scientists is circulated back to the computational scientists to realize high-level design and rapid development of chemical reactions. We hope to establish the new academic field “CReDD” which will allow efficiently developing advanced chemical reactions and materials. The integrated research on “CReDD” should lead to the development of highly efficient chemical reactions that should afford high-value-added chemicals with applications in agro- and environmental chemistry, pharmaceutical and materials science, medical technology, as well as energy and resource management. The target reactions and molecules are carefully selected based on the impact to the society through discussion among broad research communities and with many companies.

Access



Contact information

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[Facebook] https://www.facebook.com/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 drive to build within Japan “globally visible” research centers that boast a very high research standard and outstanding research environment, sufficiently attractive to prompt frontline researchers from around the world to want to work in them. ICReDD was selected as a new center of the WPI and launched in October 2018.

2019.6

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

In-depth understanding and efficient development of chemical reactions

wpi World Premier International Research Center Initiative

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