Hokkaido University Institute for Chemical Reaction Design and Discovery (ICRD)

Director
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Prof. Maeda proposed the idea of applying a virtual mechanical force to reaction systems in order to unveil potential pathways (artificial force induced reaction; AFIR). Based on this idea, he developed the world's first general method to systematically predict unknown reaction paths. We here aim to establish the scientific field of "Chemical Reaction Design and Discovery (CRD)", which should allow the efficient development of chemical reactions through a combination of computational, information, and experimental sciences.

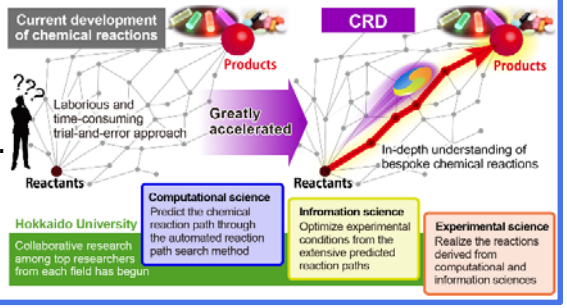
Aim

The ultimate goal of the Institute for Chemical Reaction Design and Discovery (ICRD) is to acquire an in-depth understanding of chemical reactions by analyzing complex networks of chemical reaction paths in order to accelerate the efficiency of the development of new chemical reactions. Considering that the current trial-and-error approach to the development of new chemical reactions is time-consuming and inefficient, by using state-of-the-art reaction path search methods based on quantum chemical calculations and collaborating with information and experimental scientists, we hope to establish the new academic field "Chemical Reaction Design and Discovery (CRD)", which will allows efficiently developing advanced chemical reactions and materials.

Research

The ICRD uses the AFIR method to calculate chemical reaction-path networks, 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. 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.

1. To create high value-added reactions useful for society.
2. To develop new materials based on chemical reactions.
3. To design and discover cellular and biological reactions for applications in advanced medical care.



Characteristics

- To establish the new academic field "Chemical Reaction Design and Discovery (CRD)" 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.
- 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 CRD.
- To implement organizational reform of the university centering on the establishment of the new graduate school "Chemical Reaction Design and Discovery".

Collaborations

MANABIYA system: Young researchers and students from domestic and overseas collaboration institutes stay at the ICRD for about three months, master 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 researchers, which will support the further development of this new field.