

# World Premier International Research Center Initiative (WPI)

## Summary of Research Center Project

\* Compile in English within A4 2 pages.

**Center name:** Institute for Chemical Reaction Design and Discovery (ICReDD)

**Host institution:** Hokkaido University

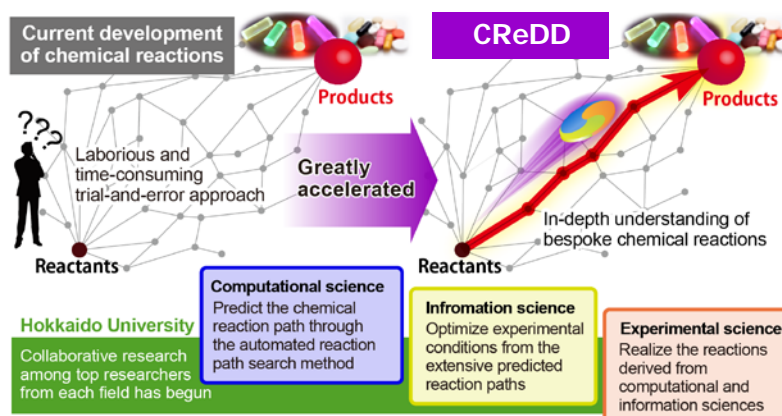
**Head of host institution:** Toyoharu Nawa (President)

**Prospective center director:** Satoshi Maeda, Professor, Faculty of Science

**Prospective administrative director:** Yasunori Yamamoto, Specially Appointed Associate Professor, Faculty of Engineering

### 1) Overall Framework of the Center Project

The ultimate goal of the Institute for Chemical Reaction Design and Discovery (ICReDD) 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. These new chemical reactions will generate advanced materials and reduce the use of energy and natural resources, which is indispensable for a prosperous and sustainable future of humanity. We aim to accomplish this objective in a research environment that integrates computational, information, and experimental sciences. Considering that the current trial-and-error approach to the development of new chemical reactions is time-consuming and inefficient, new methods for the development of bespoke chemical reactions should be a key factor toward revolutionizing the entire field of science. 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 (CReDD)", which will provide substantial knowledge on chemical reactions that allows efficiently developing advanced chemical reactions and materials.



### 2) Content of Research

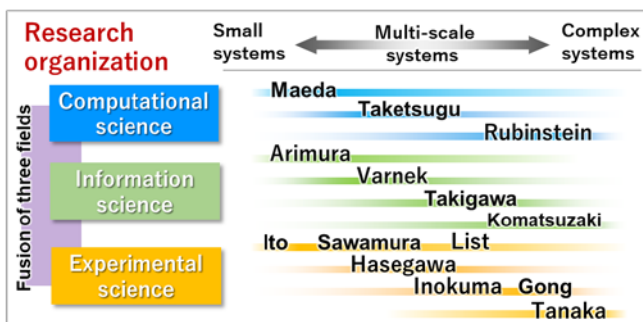
The development of new reactions by CReDD can be subdivided into three categories, depending on the size of the target molecules. The 1<sup>st</sup> category aims to create reactions that add high value to abundant and/or inexpensive resources (small molecules; ~100 atoms), e.g. synthesis of amino acids from CO<sub>2</sub>. The 2<sup>nd</sup> category is concerned with the synthesis of high-tech materials (macromolecules; ~10,000 atoms), e.g. synthesis of highly efficient light-emitting materials and ultrahigh-strength carbon materials for space elevators. In the 3<sup>rd</sup> category, CReDD will be used to investigate cellular and biochemical reactions, and some of the materials developed in the 2<sup>nd</sup> category will be used in advanced medical care (complex molecules; > 10,000 atoms), e.g. for the establishment of new diagnostic tools and treatment strategies. In collaboration with information science, Prof. Maeda's automated reaction path search method (AFIR) can be used to identify optimal synthetic paths to target structures. The real material that is significantly important and desired by human society will be synthesized by experimental scientists on the basis of the theoretical prediction.

### 3) Interdisciplinary Research

AFIR allows the extraction of the molecular behavior that is crucial for chemical reactions. Still, when AFIR is applied to more realistic systems, the time required to carry out the necessary complex calculations is relatively long. This obstacle could potentially be circumvented using established methods in information science (e.g. high-speed algorithms), which should dramatically reduce the time and cost for these

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calculations. Subsequently, experimental scientists will carry out the practical verification of the proposed reactions, and the experimental results will be analyzed and used as data feedbacked for the information scientists to extract new insights and apply these to the chemical reaction design. The success of CReDD would not only benefit areas that are directly related to the chemical industry, but also the global environment, life sciences, and society in general. The CReDD should thus act as an initiator and incubator for rapid, productive, and innovative research based on chemical reactions that affect all aspects of society.



## 4) International Research Environment

Three world-leading researchers from foreign research institutes have been invited to participate in the ICRReDD. Research groups will be established for foreign PIs, and **Co-PIs** and research staff will be employed to support and manage the research groups in close collaboration with the foreign PIs, given that the latter will also serve at their home institutions. Recruitment at the ICRReDD will be based on a competitive, international selection process, and **~30% of the researchers will be foreign**. We will establish an international hospitality support system for foreign researchers. Hokkaido University has already established **the Global Institution for Collaborative Research and Education (GI-CoRE)**, which consists of several centers. Among these, especially the Soft Matter GI-CoRE and the Information Science GI-CoRE will be incorporated into the ICRReDD as key sub-organizations. **We aim to establish the MANABIYA (an old Japanese word for "school") system** in the ICRReDD to educate young researchers and graduate students on collaborative research that integrates computational, information, and experimental sciences in order to realize a global circulation system for world-class scientists in the integrative research area CReDD. We will build a broad collaboration network through the ICRReDD research.

## 5) Center Management and System Reform

**Project management:** The director, Prof. Maeda, will serve for a minimum of 10 years, seconded by the vice director, Prof. Ito. Decision-making rights regarding central matters of institute management (e.g. recruitment and budgetary discretion) will rest exclusively with the director of the ICRReDD. Depending on the progress of research, the roles of each PI will be reviewed and evaluated periodically by the director, and appropriate incentives and/or replacements will be implemented. Dr. Yamamoto, who has extensive experience in collaborative industry research and intellectual property management will serve as the administrative director. With URA support from the headquarters, the ICRReDD will function as an organization directly connected to the university administration. The research support department will create a research environment that allows researchers and students to engage in their research without administrative interruptions.

**Research environments and establishing an independent research center:** A collaborative research space including the MANABIYA system and the Inter-science Café space will be installed in the Creative Research Institution building (CRIS). The CRIS Global Facility Center will manage instruments purchased at the ICRReDD. Using the support system of each PI's affiliated department will reduce the burden of administrative work for the PIs and ensure that research and education is their prime concern. At the launch, the ICRReDD will have secured operational funding from the university that is at least equivalent to the WPI grant. CReDD and MANABIYA will eventually be transformed into **the new "Graduate School of Chemical Reaction Design and Discovery"**. We will also create a permanent organization for the acquisition of private funding by e.g. hosting researchers from industry and establishing research consortia. The ICRReDD will incorporate research areas beyond its three core fields, such as humanities and social sciences, which are required for the promotion of research and the reformation of CRIS. By sharing new management systems acquired through the WPI, the ICRReDD will finally contribute to the reorganization of the University.