Outline of Selected Projects

Host institution	Hokkaido University
Center name	Institute for Chemical Reaction Design and Discovery
Head of host institution	Toyoharu Nawa
Prospective center director	Satoshi Maeda

<Project Summary>

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, the ICRD 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. 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. Thereby, we hope to establish the new academic field "Chemical Reaction Design and Discovery (CRD)", which will allow efficiently developing advanced chemical reactions and materials.

We also aim to establish the MANABIYA system in the ICRD 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 CRD. We will build a broad collaboration network through the ICRD research.

<Remarks>

The proposal sets out to integrate computational science, information science, and experimental science, which is expected to produce excellent synergy for broad-ranging applications.

The MANABIYA system seems to be a good way to train young scientists while increasing worldwide knowledge about the center and its research.