Realization of common platform technologies, facilities and equipment that create innovative knowledge and products

High-Dimensional Chemical Reaction Exploration Platform Transforming Material Discovery into Value Discovery

Project Leader : Toshiaki Taniike Professor, Graduate School of Advanced Science and Technology, Japan Advanced Institute of Science and Technology

R&D Team : National Institute for Material Science (NIMS), Hokkaido University, National Institute of Informatics



Summary :

The realization of a carbon-neutral society requires the innovation of catalytic technologies that synthesize fuels and chemicals from raw materials such as water, carbon dioxide, and biomass. This research aims to establish a "reaction exploration platform" that efficiently discovers new values from vast unknown spaces, replacing traditional catalyst development based on causal relationships. The reaction exploration platform is a technology that simultaneously discovers new reactions and catalysts by efficiently exploring unknown spaces. In traditional approaches, a specific reaction exists first, followed by the development of a catalyst for it. However, this research enables the exploration of both unknown and catalysts through high-throughput reactions feature experimentation and engineering, with exploration efficiency further enhanced by the introduction of autonomous techniques and optimized search algorithms.

