MI^2I: Materials research by Information-Integration Initiative

Overview

The Center for "Materials research by Information Integration" (CMI²) of MaDIS, NIMS has been entrusted with a Japan Science and Technology Agency (JST) project called "Materials research by Information Integration" Initiative (MI^2I), which started in July 2015 and will last for five years. MI^2I creates a system of industry–academia–government collaboration over a wide range of areas, from materials science to information and mathematical sciences. It also promotes the participation of companies from various fields to create an open innovation hub for data-driven (information-integrated) materials research, so called "materials informatics".

The basic idea of the innovation hub is described below as quoted from the JST homepage.

Innovation Hub, JST

Points of the Program

■ To Strengthen Functions of National Institute through Construction of "Innovation Hub" （Reformation of R&D System）

■ To Create a place where People from the Industry and Academia can Join at the point that a Core National Institute can provide as Research Functions and Infrastructure

■ To Strengthen Functions of Innovation Creation Aiming at Systemization and Technology Integration. Also, to Contribute Human Resource Development

What can be achieved at MI^2I

☐ **Construction of Innovation Hub by Functional Incorporation of Researchers and Engineers from the Industry and Academia** （Reformation of Functionality of R&D System）

☐ **Construction of Innovation Hub by Integrating Academic Fields of Materials Science and Data Science** （Reformation of Academical R&D System）
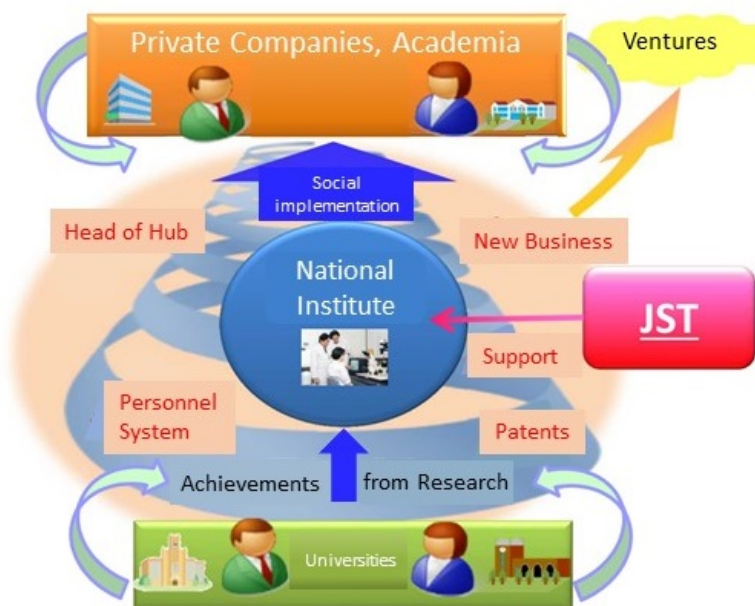
HUB of Hubs／like『Provincial Temple』system

Figure-1, Overview of Innovation Hub Program of JST
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MaDIS
NIMS MATERIALS DATA and INTEGRATED SYSTEM

NIMS 国立研究開発法人 物質・材料研究機構
National Institute for Materials Science

Objectives

◆ Rapidly develop and provide effective solutions by using data-driven materials science to meet the materials research challenges of industry and academia.

◆ Develop the tools needed for new materials development packages by using AI technologies, leading to innovations in materials research and development.

◆ Develop and improve a database available to both industry and academia and construct a data platform(DPF) for a new materials development approach, which will be Japan's potential intellectual assets in conjunction with the above-mentioned tools.
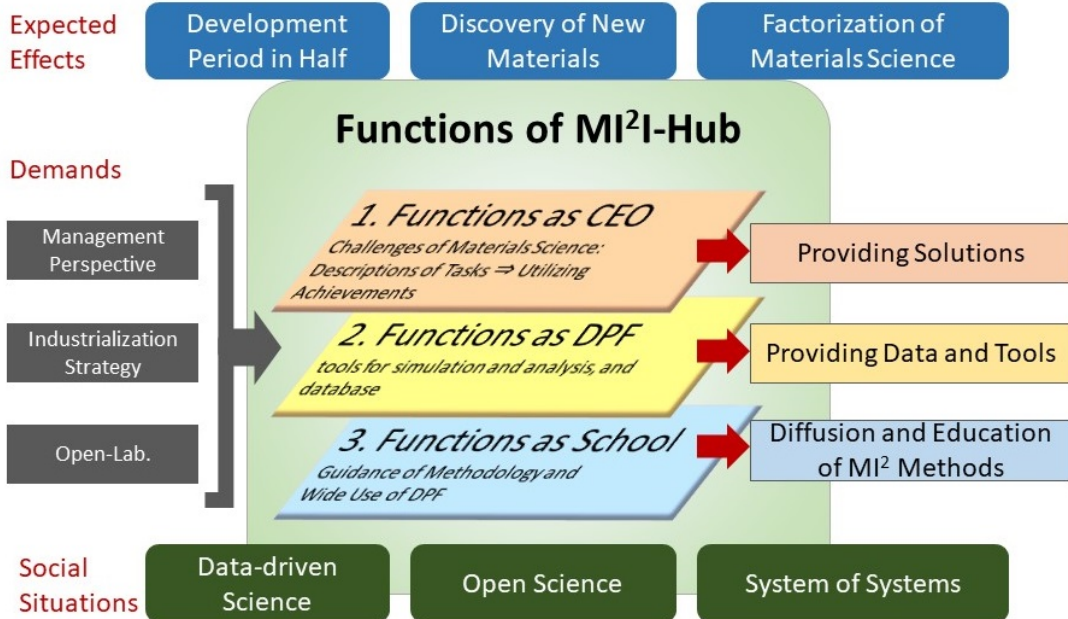
Figure-2, Three-Layer Structure and Functions of MI²I-Hub

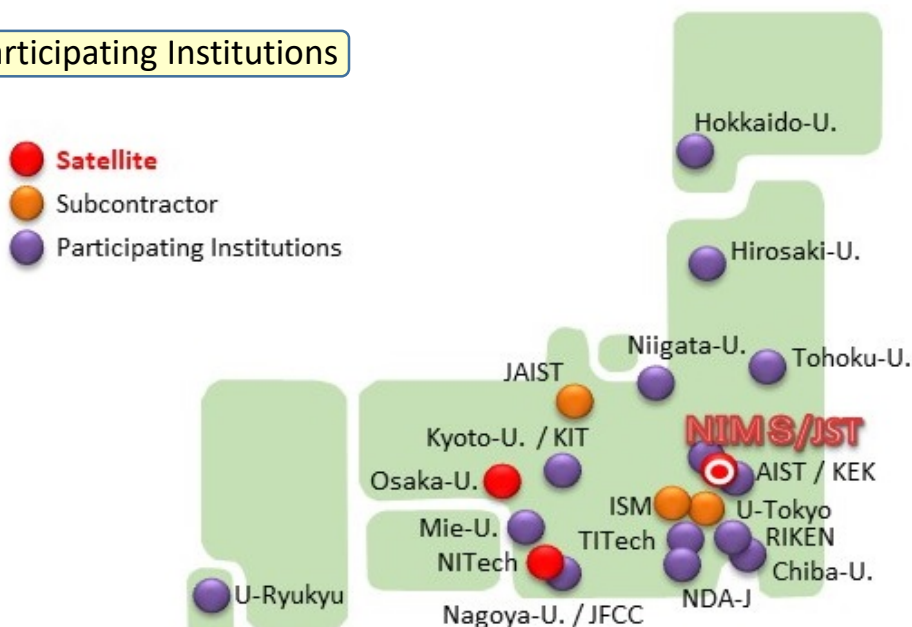## Major Participating Institutions

Figure-3, Participating Institutions

Research Organization

 The research organization of MI²I is shown below in Fig.4. The basic idea behind this organization lies in its three-layer structure. Three important themes of materials science, rechargeable battery materials, magnet materials and thermal management materials, all of which are related to energy and environmental problems, are set in the top layer. The characteristic aspect of MI²I is that these targets are pursued not only with the traditional approaches, experiment, theory and computational science, but also with data science, the fourth paradigm, which is located in the middle layer. Materials descriptor platform is obviously related to data science. Topological analysis is a new powerful approach for characterizing complex materials structure, and materials exploration is a task common to the three themes in the top layer. The first layer activities form columns and those in the second layer form rows, so that their crossing parts represent collaboration.

 Through these activities, we are creating Data Platform, an information-integrated system for materials discovery and development that is available to researchers and engineers from industry, academia, and government. The materials database that NIMS has been developing and improving over the years plays an important role in this work, and we intend to enrich the database and improve its usability.
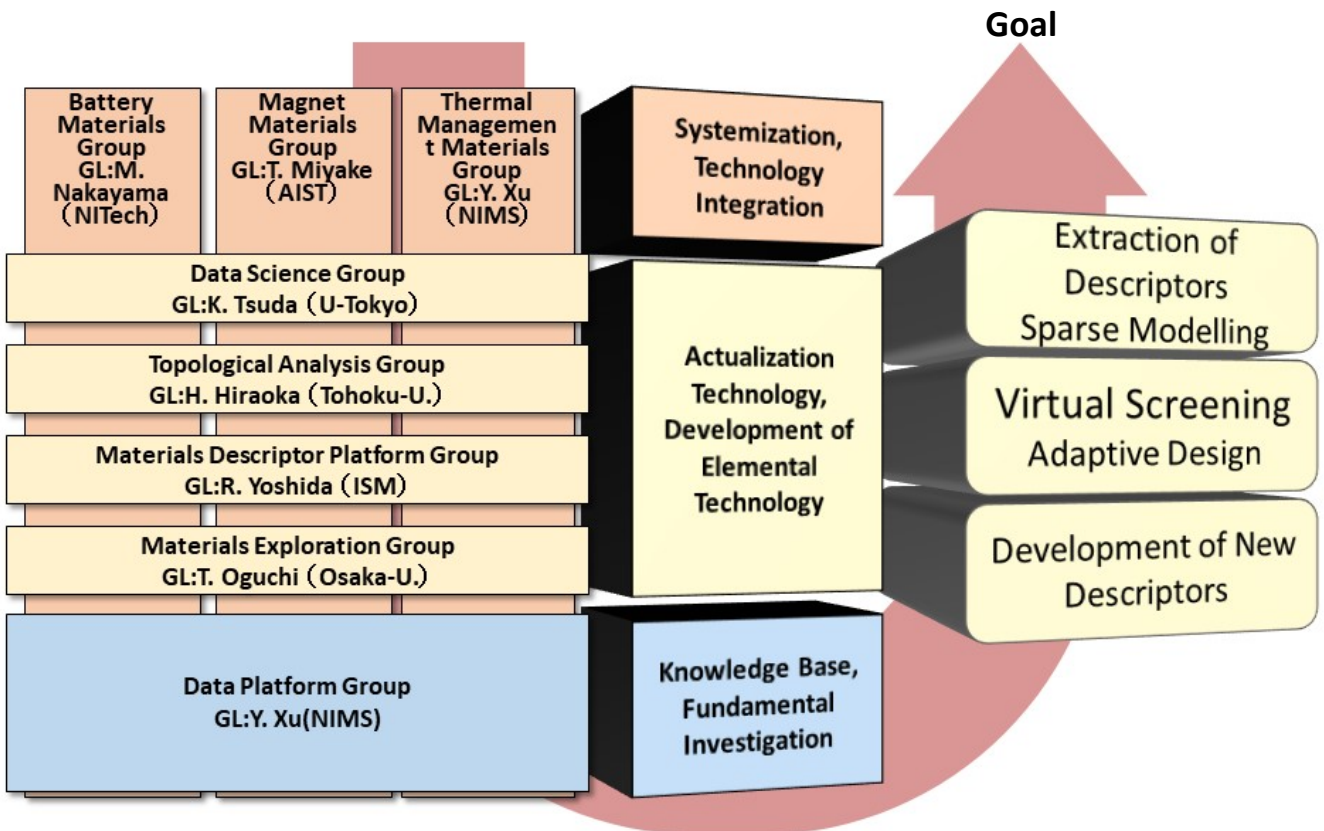

Figure-4, Three-Layer Research Organization and Goal Settings

Personnel

Executives and Advisor

Project Leader
S. Itoh
NIMS

Program Manager
N. Kihara
JST

Sub Proj. Leader
T. Chikyo
NIMS

Sub Proj. Leader
A. Manabe
NIMS

Sub Proj. Leader
M. Okada
Tokyo Univ.

Executive Advisor
K. Terakura
NIMS

Research Group Leaders

Battery
Materials
M. Nakayama
Nagoya I. T.

Magnet
Materials
T. Miyake
AIST

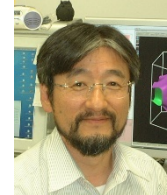Thermal Manag.
& Data Platform
Y. Xu
NIMS

Data Science
K. Tsuda
Tokyo Univ.

Topological
Analysis
H. Hiraoka
Tohoku Univ.

Mater. Descriptor
Platform
R. Yoshida
ISM

Materials
Exploration
T. Oguchi
Osaka Univ.

Events

The 6th MI²I Forum will be held on Feb 21st, 2018 at Hitotsubashi-hall in Tokyo.
The progress of MI²I activities will be reported and more than 20 poster presentations will be provided. Dr. K. Terakuka of MI²I EA and Dr. T. Shoji of TOYOTA MOTOR Corp. will also give lectures.

> ➤ MI²I Letter will provide News and Report of MI²I activities in the coming issues.
> Particularly, method and software developed in MI²I will be explained. They include
> 1) "COMBO: COMmon Bayesian Optimization (efficient Bayesian optimization)",
> 2) "qspr and iqspr for molecules (Bayes theorem + natural language processing)" ,
> 3) "MDTS (Materials Design by Monte Carlo Tree Search)",
> and so on.
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