Research area in Strategic Objective "Construction of revolutional material development methods through fusion among experiments and theory/data science"

6.1.3 Revolutional material development by fusion of strong experiments with theory/data science

Research Supervisor: Hideo Hosono (Professor, Institute of Innovative Research, Tokyo Institute of Technology)

Overview

This research area merges theory, computation, and data science with the experimental sciences, which has been the basis of substance and material development undertaken so far, with the aim of building methods for revolutional material development. Specifically, this research area focuses on the realization of materials or functions that have great societal need but has not yet been achieved, through new research teaming and techniques, thus demonstrating a new integrative approach of Japanese materials research, which has been leading the world so far. This research area not only covers materials science but also involves a complex system, which is essential for the development of real materials.

The system comprises theoretical, computational, and data researchers centered on an experimental materials science system to promote research in close collaboration with them.

This research area offers revolutional and novel methods for materials development to promote industrial competitiveness in our country.

Research Supervisor's Policy on Call for Application, Selection, and Management of the Research Area

Background

Progress in informatics technology and computer simulation has ushered materials research and development into an era of revolution, wherein the active use of these technologies has expedited the search for new materials, resulting in a number of achievements in this field. On the other hand, theories and modeling tools used for describing the behavior of existing substances are not adequately available for materials synthesis or property control, which impedes revolution.

Considering the trend overseas, the U.S., which leads the Materials Genome Initiative, has invested 500 million dollars in five years since 2011, whereas the European countries such as Germany, Switzerland, and Spain have promoted various projects. Nearer home, China has established Shanghai Materials Genome Institute on the campus of Shanghai University. In other words, countries are vigorously undertaking human resource development and research in various phases.

On the other hand, Japan has produced many researchers with remarkable achievements and strong experimental materials research skills in the synthesis sector suitable for materials and in the process sector, which involves trial manufacturing and production of targeted materials by controlling the textures, who have achieved high international positions. However, foreign countries are progressively investing in research and development as well as human resources, which make it increasingly difficult for the sustainability of the research sector in Japan against international superiority without revolutional research and development methods.

For a persistent production of revolutional materials that would lead the world in the future, Japan needs to take advantage of its characteristic strength in experimental research to expedite its development. It is urgent for Japan to introduce rapid improvement in computer performance and progress in informatics technology in a coordinated manner in order to build its own characteristic new methods for the development of new materials.

Policies for proposal invitation and selection

This research area merges the strong experimental science with the theoretical, computational, and

data sciences to promote the research and development of new materials. Materials and processes are not restricted but cover a wide range of fields including inorganic, organic, metallic, functional, and structural materials. Research proposals that can yield materials are invited.

Positive evaluations would be given to those proposals that use revolutional methods of computational science or data science based on condensed matter theories. Theoretical computation includes first-principles calculation, numerical simulation, and the like. Data science is represented by machine learning, Bayesian inference, sparse modeling, and data mining. Topology and graph theory are examples of mathematical approach. We encourage not only the improvement of existing methods but also the development of original new methods.

The proposal is required to describe clearly condensed matter theories, computational science techniques, mathematical approach and/or data science techniques, that can be used in combination with the experimental sciences, and then comment on the originality and strength of the collaborative team. We welcome team compositions that are clearly different from conventional material research systems and suitable for pioneering in the frontiers of material research.

Because the essence of research output is a “material”, collaboration with an excellent experimental researcher is mandatory although the research team representative need not be an experimental researcher.

Because this research area seeks new material development methods that do not exist, it welcomes challenges by energetic researchers with high potential, preferably not established, who can promote the development of original materials.

Managing policies for the research area

The research supervisor imposes the following conditions on the researchers participating in this research area:

(1) Flexible modification of the research team or research plan upon review

(2) Collaboration with researchers and engineers within and without the research area

(3) Promotion of the development of young human resources for research

(4) Mandatory collaboration with industries after mid-term evaluation

(1) Flexible review of the research team or research plan

When the research supervisor finds that a proposed research team needs to be strengthened or that it

might be useful to merge a proposed technique with a different technique or material, he/she can instruct to alter the research plan. Follow the instruction to promote joint research or review the team composition.

(2) Collaboration with researchers and engineers from within and without the research field

Researchers participating in this research area are requested not only to yield materials but also to promulgate the techniques and effects of the collaboration widely. For this purpose, they may be requested to cooperate with researchers and engineers within and without the research area for the promotion of collaboration.

(3) Undertaking the development of young human resources for research

Researchers, engineers, and students participating in this research area may be expected to become well versed in experimental sciences and updated theoretical, computational, and data sciences through the collaboration for their growth as human resources who can promote the development of revolutional materials. Therefore, this research area emphasizes the innovation of research and development methods to yield human resources who can support science and technology in Japan in the future.

As research progresses, this research area would promote collaboration and cooperation with the research projects such as the “Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences” and “Development and application of intelligent measurement-analysis methods through coalition between measurement technologies and informatics” of JST PRESTO, and the “Materials research by Information Integration Initiative” of the nanotechnology platforms of the Ministry of Education, Sports, Culture, Science and Technology and the SIP “Structural Materials for Innovation”.

○ This research area sets the maximum amount of initial research expenses for CREST at a total of approximately 300 million yen (excluding indirect expenses).