Research area in the Strategic Objectives "The invention of innovative catalysts using diverse natural carbon resources", "Creation, advancement, and systematization of innovative information technologies and their underlying mathematical methodologies for obtaining new knowledge and insight from use of big data across different fields", "Creation of new functional materials by means of technology for controlling spaces and gaps in advanced materials in order to realize selective material storage, transport, chemical separation, and conversion, etc.", and "Establishment of molecular technology, which is the free control of molecules to bring innovation to environmental and energy materials, electronic materials, and health and medical materials"

6.2.12 Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences

Research Supervisor: Shinji Tsuneyuki (Professor, School of Science, The University of Tokyo)

Overview

Through the high-precision knowledge obtained through progress in measurement and analytical techniques, advances in combinatorial synthesis and other high-throughput experimental approaches, dramatic improvements in computing capability, first-principle calculation and other powerful computational science, understanding of the principles of materials science is advancing, and large amounts of related data is being obtained in a short time. In addition, some areas of information technology are making remarkable progress in extracting meaning and new knowledge from this large amount of complex data.

In this research area, we aim to establish advanced materials informatics platform tackling new materials design using knowledge obtained through the collaboration and merger of experimental science, theoretical science, computational science, and data-centric science, using the strengths of each approach. We also aim to produce young research leaders who can perform on a global level in future.

Specifically, this includes the following research;

1) Promotion of the discovery of new materials that will realize functions to meet social and industrial requirements, and establishment of guiding principle for materials design
2) Development of inductive methodologies clarifying structure-property correlations and physical law from large-scale, complex data, and discovery and design of novel materials using them
3) Establishment of high-throughput screening of candidate materials that will contribute to high-precision forecasting of the physical properties of unknown substances and experimental design of synthesis and evaluation
4) Development of new physical concepts and methodologies to comprehensively describe, store, and visualize diverse materials data
5) Development of data acquisition, storage and management technology that will contribute to the integration of

data-intensive science and materials science, and maintenance of databases, and development of tools for various statistical analysis, machine learning, visualization, etc.

We aim to promote pioneering and innovative research that will dramatically accelerate the materials design and discovery to contribute to many industrial applications in energy, medicine, chemistry and so on, stimulating a paradigm shift in materials science.

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

1. Background

Materials have latent functions that far exceed human imagination, and competition is heating up globally to discover and put them to use with science and technology. The research and development of new materials is a source that supports various industries and the evolution of society, and continuously promoting this development is necessary in order for Japan to grow and advance into the future. In addition, the discovery of high temperature superconductors has caused the physics of strongly-correlated electrons systems to flourish, and as development trends towards devices based on new operating principles, the discovery of novel materials represents a cradle for the progress in basic science as well as the development of innovative technologies based on scientific knowledge.

In recent years, in the field of materials science, measurement and analytical techniques that enable unprecedentedly sophisticated analysis of composition and structure, combinatorial synthesis and other high throughput experimental approaches, first-principle calculation and other numerical approaches enabled by high-performance computer, have driven the interaction among the so-called first, second and the third paradigm of science, resulting in rapid advances in the development of materials science.

However, when aiming to design materials with specific functions, the determination of precise element composition and stable structures from an enormous range of possibilities presents a very difficult task. Even if a candidate substance is specified, the material structure and its characteristics will differ according to the manufacturing process, so materials development is a very empirical trial-and-error situation based on experience and intuition.

On the other hand, there are some areas of information science and technology making remarkable progress in extracting meaning and new knowledge from large amounts of complex data. Analysis of large amounts of data obtained by high-throughput synthesis and large scale simulation and so on, given meaning with knowledge from materials science —in other words introducing fourth paradigm data-centric science—is expected to provide unprecedented new knowledge, leading to breakthroughs in materials research and development.

(2) The required research

With this background, in this research area, we aim to establish advanced materials informatics tackling new

material design using knowledge obtained through the integration of experimental science, theoretical science, computational science, and data-centric science, using the strengths of each approach. We also aim to produce young research leaders who can perform on a global level in future.

Specifically, we are assuming research examples such as those shown in Outline of the Research Area 1) to 5), but not necessarily restricted to those topics. We expect challenging research that will bring about significant impact in future materials design.

The targeted materials include organic and inorganic compounds, metals and alloys, high polymer compounds, and amorphous substances. In fact, we encourage the selection of comprehensive candidate materials with a reverse design concept of making chemical compositions, crystal structures, electronic states, synthetic methods, microstructures and so on, taking the required functions such as electromagnetic, optical, thermal, reactive, mechanical strength and other characteristics as a starting point.

In the proposal, it is desirable to include the impact on science and technology arising from the materials development, the new knowledge that can be expected to be obtained from the proposed method, the functions of the new materials, and the contribution to industry society.

We are requesting proposals for achieving dramatic rationalization of material development time and cost through the discovery of new materials with the desired functions, a deeper understanding of the principles of properties expression, and systematic materials design that surpasses trial-and-error know-how.. We hope for challenging proposals based on fresh concepts that do not simply follow previous research from overseas, and we are seeking research that will give Japan a continuous edge in global competition.

(3) Recommending Collaboration with Other Research Areas

This research area includes many goals, which cannot be achieved by conventional singular disciplines such as physics, chemistry, and materials engineering, which had investigated the field of materials science in the past but for which collaboration and merging with the fields of informatics, statistics, and mathematical science is inevitable. In preparing the research proposal, we expect improvement in specific and realistic research proposals consequent to discussions among experts in dissimilar fields. There is also the possibility that issues and solutions that had been overlooked as preparation was conducted only from the viewpoint of one research proposer will be discovered. In light of this, this research area strongly recommends that the contents of proposals be deepened through discussion with experts who have different knowledge and skills from the proposer.

Following the last fiscal year, we are accepting research proposals (collaborative proposals) that involve collaboration with other researchers. However, since PRESTO projects are research projects pursued by individual researchers, evaluations regarding selection are based on individual research proposals. It is up to the proposer whether they include a collaborative proposal in their research proposal. Inclusion will not directly affect the evaluation of proposals to be selected. However, we are planning to recommend collaborative research with respect to the contents indicated in the proposal as an effort to promote the research area following selection. If you intend

to include a collaborative proposal in your research proposal, please specify which part the proposer will be in charge of and what will become possible that cannot be achieved by individual research alone.

(4) Activities in the research area after adoption

While collaborative proposals as in (3) above are possible, we will also actively support cooperation after selection that is deemed necessary for the research area. In addition, we will also promote collaboration with various research projects in Japan and overseas including related CREST and PRESTO research areas. Furthermore, we intend to promote open science such as sharing data and data analysis tools together with other projects. It is required to formulate a data management plan after adoption (please refer to “Chapter 3.3.5 (6)).

* Please note that the application forms of this research area are different from those of the other research areas.

Time & Date	Venue
April 21 (Fri) 13:00-14:30	< Kansai-Area > TKP Garden-City Kyoto (Kyoto Tower Hotel) 2F “Suiren ”
April 24 (Mon) 13:00-15:00	< Kanto-Area > Tokyo Headquarters K's Gobancho7, Gobancho, Chiyoda-ku, Tokyo 102-0076 Japan

For more information, please visit the following site: http://www.senryaku.jst.go.jp/teian-en.html