Research area in Strategic Objective "Opening up of unexplored exploration space of materials with multi-element, composite, and metastable phases based on elements strategy"

Creation of future materials by expanding materials exploration space

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Overview

The main aim of this research is to design new functional materials which will expand our fundamental knowledges in material science. These new materials are expected to be originated from simple but original ideas, and potentially prepared by using unconventional techniques. These new materials, together with the new designing principles, will help us solve challenges this society is currently facing, including but not limited to issues in areas of environment, natural resource, energy, medicine and health.

Specifically, the project will focus on the synthesis and characterization of materials strongly related to energy, electronics, medicine and environment. There are three perspectives regarding the research scheme: A scheme of 'multi-elements', in which materials containing different elements will be synthesized and investigated to understand how to combine the advantages of different elements; A scheme of 'functional composites' in which one will study how compositions/configurations of different elements in new materials affect the functionalities; A scheme of 'metastable phases', in which careful kinetic control will be employed to produce metastable materials.

In addition, the project aims to realize new synthetic pathways and designing principles (new theories) into 'future functional material'. Aim for research with a challenging approach backed up by a broad perspective, including the construction of principles by combining these with computational science, data-driven science such as machine learning, cutting-edge operand measurement techniques, and more, in order to establish technology for materials creation synthesis techniques and process control techniques.

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

1. Basic concept

The proposed research should target in the development of unknown materials exploration space and the foundational techniques to support this, with the goal of creating future materials that express novel

and unexpected functions that will change the essence of a materials science. By greatly expanding the scope of the exploration of materials, these materials are expected to possess higher efficiency and/or better functionalities with respect to their current counterparts, combine multiple functionalities, and/or balance the contradictories originated from different functionalities. Furthermore, theoretical/computational study, which helps understanding the fundamentals in functional materials and guide the discovery of new functional materials, is welcome. Research in the development of unconventional synthetic and characterization techniques is also encouraged.

The proposed research should focus on materials in electronics, environmental science, energy, medical science and/or related areas. Proposals with simple but original ideas are particularly welcome. Although we encourage broad research proposals with high-level originality, applicants should specify their detailed plans, approaches and expected impacts in their applications.

2. Assumed research fields

This project is looking for ideas which produce new visions and concepts in functional materials. Consequently, research proposals that extend conventional routes, such as those that simply optimize materials or improve existing processes, are not eligible. The proposed research does not need to be limited in conventional material science fields (such as inorganic and organic chemistry, metallurgy, composite materials, material characterization and etc.). Although three perspectives (multi-elements, functional composites and metastable phases) are listed in Overview, these are guidelines and researches focusing other specific areas are also welcome. In addition, regarding developing synthetic methods towards new materials, they are not restricted to focus on simple solids, liquids and gases. We broadly welcome proposals which aim to solve the general challenges related to social problems. The following specific research projects are shown as examples:

1) The creation of new materials that make practical use of multi-elements, functional composites, metastable phases, and more by combining elements after understanding the synergy effects of different elements with each other

• The development of materials made from multi-elements that surpass conventional single-element, two-element, and three-element.

Multi-elements alloys, solid electrolytes, thermoelectric, high-entropy alloys, macromolecules containing heterogenous elements, etc.

• The development of materials that express functions through interface control, accomplished by combining different types of elements and structures

Hydrogenomics, mixed- anion compounds, composite catalysts, etc.

• The development of materials that make practical use of thermodynamically unstable metastable phases, etc.

High- temperature superconductivity, power semi-conductors, glass macromolecules, etc.

- 2) The construction of foundational techniques that will support the creation of new materials
 - · Theories and computational science

Exploring and controlling reaction paths, materials informatics, etc.

· Data science and high-precision processes

High throughput experiments, multi-element exploration systems (AI robots), process simulations, etc.

· Measurement and evaluation techniques

Operand measurement, multiscale and multimodal measurements, observation of atomic resolution, etc.

3. Points to note when apply

When you apply, although we do assume that you will achieve your plan during the PRESTO work period, we expect selected researches to make a social impact in the near future. Please note despite the individual proposal, you do not need to cover all the research contents by your own, and a jointresearch is allowed, in which case, please describe the joint-research plan specifically. Due to the fact that the review panels include scientists with different backgrounds, please describe your plan in a way that people outside your fields are able to understand the originality, significance and impacts of your research. Please note we consider not only the direct impact of your research during the project period, but also the potential future developments originated from your research after that period.

This PRESTO project is individual. The expected total research costs will be 30-40 million yen (direct costs). The project will cover a period of 3 years and 6 months.

4. Management Policies

We are determined to build a friendly environment for researchers. The required time for obtaining results depends on the nature of proposed research. However, you must setup a reasonable schedule during PRESTO research period. This schedule should consider future plan even after the PRESTO period. In order to help exchange ideas, facilitate collaborations, and maximize the impact of this project, meetings between researchers will be arranged twice a year, laboratories in which researcher are based will also be visited. We respect diversity in terms of research institutions, regions, gender, etc., to maximize the appeal of researchers and research topics, to value synergy among researchers connected by "dreams," to produce research from new perspectives and flexible ideas. The entire research field will be supported so that researchers can envision their own future. Through the promotion of this research field, we hope to nurture the next generation of leaders in materials creation.

There will be additional workshops, symposiums and other meetings with overseas institutions. The project will also be collaborated with CREST's 'Exploring Innovative Materials in Unknown Search Space'.