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

Exploring Innovative Materials in Unknown Search Space

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Overview

This research area aims to create new materials with innovative functions by drawing out the latent potential of chemical elements to the fullest extent through the synergy of multiple elements. More specifically, we are expanding materials search space into unknown areas, such as multi-component compounds, multi-element systems, and metastable phases, regardless of whether these materials are inorganic or organic. We are emphasizing strategic initiatives that will promote efficient materials searches.

Regarding multi-component compounds, new molecules and solid materials made by undeveloped combination of elements, or nanosystems formed with heterogenous junctions or building units may realize innovative functions. In terms of multi-element system, one may discover a variety of new phases (e.g., crystalline phases, amorphous phases, electron phases, and spin phases) and design materials positively using diverse types of defects. As for metastable phases, one may develop new materials through kinetic-control processes or nonequilibrium synthesis, realize desired crystalline phases and physical properties, enhance ion diffusion, battery capacity, and catalytic reaction, and control reversible phases. Also, one may even discover simple and useful materials like the allotropes of carbon (fullerene, diamond, ---). Other than the above, we welcome new concepts for designing materials, for example, informatics that adopt human insight, intuition, and sensitivity.

We expect the goal of each research team to be the development of effective methods to create materials, including computational science/data science/high-throughput screening methods/nonequilibrium processes/in-situ measurements that are directly connected to informatics; proof of the development of novel functionalities or significant improvements in functionalities and durability. The outcomes of this research area will be integrated to construct the science of the advanced usage of elements and the foundation for creating new functional materials.

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

1. Basic concept

By using and applying the latent potential of elements to the utmost, this research area aims to create new materials that have innovative functions or significant performance that will contribute to solving

increasingly serious social problems. Although this has been carried out based on the “Element Strategy”, which mainly develops alternatives to rare elements, we encourage researchers to expand materials search space into unknown areas, such as multi-component compounds, multi-element systems, and metastable phases, regardless of whether these materials are inorganic or organic, and to propose concepts and methodologies for the design of new materials. Therefore, in this research area we do not expect proposals for a simple extension or simple improvement of researches on conventional methods.

To develop new materials with novel functionalities and/or significant performance in an unknown area, it is essential to have ideas for the advanced usage of elements after setting the social problem you aim to solve. Even if you present an idea based on a variety of concepts (including multi-component compounds, multi-element systems, or metastable phases) and/or an original vision, please state how it is novel, and the theories/predictions behind it. With such ideas as a starting point, it is important to pioneer methodology to search in unknown materials space, to apply or newly develop techniques to synthesize and search for different materials, and to logically describe a research strategy that goes all the way to proof of novel functions. Please clearly describe ideas and strategies on these issues in your proposal.

In FY2022, JST and ANR (Agence Nationale de la Recherche) invite Japanese-French joint research proposals in addition to regular (non-joint) ones. We welcome proposals that have effevtive strategy of leverage through the cooperation of Japanese and French researchers.

2. Assumed research fields

(1) Techniques to efficiently search for new materials in unexplored areas and (2) new processing techniques to synthesize the materials are the research points that we need to prove ideas related to the realization of innovative functions by applying elements in advanced ways.

[Techniques to efficiently search for new materials in unknown areas]

- Computational science, data science, and high throughput screening methods to predict and discover substances that can specifically display high functionality in multi-element materials and nonequilibrium materials, as represented by diamond and metallic glass
- Design methods for new functional materials systems through the building units arrangement, layering, interface, etc. of heterogenous nanolevel structures
- Design methods for materials that simultaneously fulfill multiple functions, including electron/ion transport, optical, magnetic, dielectric properties, electrochemical energy storage, chemical reactivity and catalysis
- Techniques to efficiently create phase diagrams that incorporate factors controllable in engineering (other than temperature and pressure), and state diagrams at high temperatures
- Exploring informatics that adopt human insight, intuition, sensitivity, and more.

[New processing techniques to synthesize new materials]

- New processes that precisely control the time profile of pressure/temperature/atmosphere, use plasma, ions, electromagnetic waves, solutions, etc., and occur in nonequilibrium, at low temperatures, and/or under extreme conditions
- Techniques to control aggregation and local reactivity so that multiple nanolevel structures can be arranged adjacently
- The advancement of methods to control mechanical stress in thin films grown on special substrates
- Collaboration between data science techniques and operands/in-situ measurements that locally assess the structures and physical properties of the synthesis fronts, etc.

Moreover, in order to actually and widely use the developed materials, we must also consider:

- Life-span, increased durability, the stabilization of metastable phases, etc.

This research area accepts all materials fields, including inorganic, organic, and metal. It is also not limited by the shape of materials, such as crystal/non-crystal/solid solutions/flexible/soft materials. Although we have brought up multi-component compounds, multi-element system, and metastable phases as sample categories, other material categories in unknown areas are also considered eligible for research and development. However, simply improved research on existing materials via conventional methods, and proposals that are only extensions of past research are not eligible. Please submit proposals for research projects with free concepts that are not constrained by conventional Element Strategy or common sense, and clarify the novelty of your idea for the advanced application of elements, and your strategy to realize it.

3. The organization of research teams

With the aim of creating new materials and novel functions, in this research area we are encouraging the formation of teams made up of groups that are responsible for computational science, data science, and cutting-edge measurements, in addition to material synthesis groups. Please endeavor to closely collaborate to create new materials research methods that are distinct from trial-and-error methods and simply improved forms of conventional techniques. We hope that there will be groups that specialize in high throughput experiments and operand measurements directly connected to data science within teams, but this is not necessary as an application requirement; if it becomes necessary when realizing your idea, you should consider collaborating within or outside of this research area. With regard to plans for research budgets, please set these out appropriately so that the research director bears responsibility for the results of the overall project, without allocating uniform fixed amounts to each group. Please note that proposals that focus mainly on the development of labor-saving through robotics that are not connected to nonconventional materials search techniques are not eligible.

4. Research budget and period

The upper limit of the research budget is 300 million yen (direct costs) per project. However, if the proposal is wide-ranging across, for example, computational science/data science/high throughput assessments/nonequilibrium processes/in-situ measurement directly connected with data science, and the necessity is truly acknowledged, the upper limit may be raised to 400 million yen (direct costs) per project. The research term is within 5.5 years from FY2022 to FY 2027.

Even for the JST-ANR joint proposals, the upper limit mentioned above is applied to the Japanese side team.

5. Principles of management

- A site visit will take place within about 18 months following project selection; the set-up of the research environment and research teams will be checked, and the research plan/images of concrete outcomes will be shared.
- Research area meetings will be held once or twice a year, to review research progress and, if necessary, to revise research plans/organization. Since other teams may even be interested in examples of failures from a different aim or perspective, please proactively report these in the meetings.
- Three years after research begins, an interim evaluation of your project will take place; this will assess how the project has taken on the challenge of materials searches in unknown areas. Moreover, there will be discussions about measures to expand research outcomes in the second half of the project, to promote publications such as research papers, to acquire patents, and to enhance collaboration with industry. We will also hold symposiums, where those involved will report their results to external researchers, and discuss how to expand their outcomes.
- There will be an ex-post evaluation of projects in the final year of research, in which policies to further develop outcomes after the research period is finished will be discussed. There will also be symposiums, which should demonstrate the appeals of the outcomes of your CREST research.
- Collaboration should be considered with those within and outside of this research area, especially collaboration with the PRESTO research area “Creation of future materials by expanding materials exploration space,” which was established based on the same strategic objectives.
- Excellent operands/in-situ measurements techniques should be shared and adopted by other teams within this research area and the above PRESTO research area to accelerate the development of new process/synthesis technologies.