Title of Project : Materials Science and Advanced Electronics Created by Singularity

Hiroshi Fujioka
(The University of Tokyo, Institute of Industrial Science, Professor)

Research Project Number : 16H06413 Researcher Number : 50282570

【Purpose of the Research Project】

Crystalline materials comprise periodically arranged atoms. Traditionally, any disorders found in crystals have been regarded as structural defects that ought to be eliminated from the materials. Recent progress in solid-state electronics, which has led to the explosive development of the information society, is in fact based on the crystallography and physics of these perfect crystals. However, our "singularity-structure project" is trying to introduce a Copernican revolution in this notion: it aims to focus on imperfect crystals which contain intentionally introduced defects. We are trying to understand the basic characteristics of the defects embedded in perfect crystals, which we define as "singularity structures." We would like to lay the foundations for a new discipline within crystallography and for the physics related to crystals with imperfection. Furthermore, we will try to fabricate functional electronic devices—that cannot be achieved with conventional perfect crystals—by having these devices take advantage of the versatile physical properties of singularity structures.

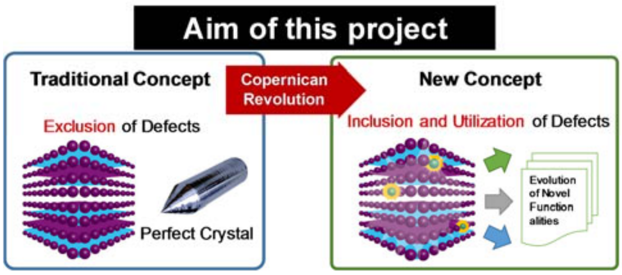

Figure 1 Basic concept of this project.

【Content of the Research Project】

This project covers various research topics such as the preparation/characterization of singularity structures, device fabrication with singularity structures, and theory for new crystallography and physics for singularity structures. This study will necessitate close collaboration among scientists from various fields, such as electrical engineering, chemistry, and theoretical/experimental physics. The work on the project will be divided into four areas:

A01: Crystal growth and construction of extended crystallography,
A02: Processing and application for novel electronics,
B01: Structural characterization of defects and their properties,
B02: Optical characterization of defects and their properties.

In addition to our own research plans, we intend to incorporate innovative ideas from young researchers by collecting their plans on all topics related to singularity structures.

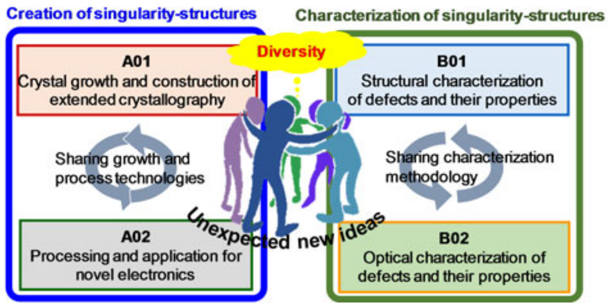

Figure 2 Organization chart of this project.

【Expected Research Achievements and Scientific Significance】

At the end of this project, our achievements will make obsolete the notion that perfect crystals are the best materials for crystallography; furthermore, we will explain that crystals with defects are the treasure houses of new functionalities. We expect singularity structures to not only be applied to conventional applications, such as lighting, communication, data processing, power control, and energy generation, but also to new fields such as agriculture, medicine, pharmacy, and chemical synthesis.

【Key Words】

Perfect crystal : Crystals that comprise in perfectly periodically-aligned atoms.
Singularity crystal : Imperfect crystals which contain intentionally introduced defects.

【Term of Project】 FY2016-2020

【Budget Allocation】 1,103,800 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Coordination Asymmetry: Design of Asymmetric Coordination Sphere and Anisotropic Assembly for the Creation of Functional Molecules

Mitsuhiko Shionoya
(The University of Tokyo, Graduate School of Science, Professor)

Research Project Number : 16H06508 Researcher Number : 60187333

【Purpose of the Research Project】

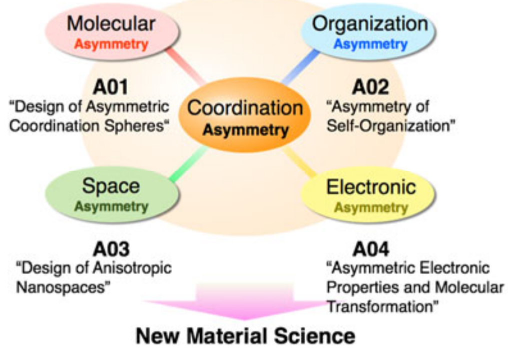
One of the final goals in chemistry is to control absolute/relative configurations of every element and to precisely design their bonding. It is therefore of key importance for developing new material science to construct metal–centered chirality and asymmetric coordination spheres.

This project aims at developing constructive methods for asymmetric coordination spheres and anisotropically assembled structures of metal complexes by theory, experiment, and instrumentation, focusing on metal elements and their coordination spheres as platforms for steric control, reactions, and functional expression. Namely, methods to create asymmetric and steric/electronic structures of metal complexes and their nano– to micron–size assembled structures will be developed by the molecule-based control of the coordination spheres to establish a scientific principle of "coordination asymmetry". In particular, constructive methods for chiral metal complexes, including asymmetric induction of prochiral metal complexes, and asymmetric assembled structures are expected to develop new molecules and materials with anisotropic and directional structures and functions. This principle would open new research comparable to asymmetric organic synthesis by making innovations for metal coordination–based advanced materials.

【Content of the Research Project】

In this research area, the following four research items collaborate closely with each other between research groups of theory, experiment, and instrumentation. A1 (molecular asymmetry): construction of asymmetric coordination spheres of metal complexes, elucidation of structure, reactivity, dynamic property of asymmetric metal complexes in solution and the solid states and at the interface. A2 (organization asymmetry): nano– to micron–size anisotropic self–assembly of coordination nanomaterials leading to assembled structure–based functions. A3 (space asymmetry): construction of asymmetric spaces based on the natures of coordination bonding directed toward amplification and dynamic control of directional and anisotropic space functions. A4 (electronic asymmetry): anisotropic assembly of coordination compounds by bridging with chiral ligands and asymmetry transfer at the interface or space directed toward asymmetric molecular transformation and chiral/directional functions.

Proposals with supportive, transversal, and applied perspectives will be openly recruited for these research items.



【Expected Research Achievements and Scientific Significance】

This project will establish a new scientific principle regarding constructive methods for coordination spheres and anisotropic assembly of metal complexes, which will result in the paradigm shift not only for coordination chemistry but also for material science. A new class of materials will be created by the precise design of absolute/relative configurations of metal complexes and their assembled materials (unit/organization design). With a view to such an essential part of chemistry and every related field, we promote this project with a principle of "coordination asymmetry".

We also focus on international collaboration between different fields leading to international network development, looking for young players to develop with a higher viewpoint and expertise.

【Key Word】
Coordination asymmetry: a scientific principle regarding constructive methods for asymmetric coordination spheres of metal complexes and their anisotropically assembled structures

【Term of Project】 FY2016-2020

【Budget Allocation】 1,168,000 Thousand Yen

【Homepage Address and Other Contact Information】
http://asymmetallic.jp
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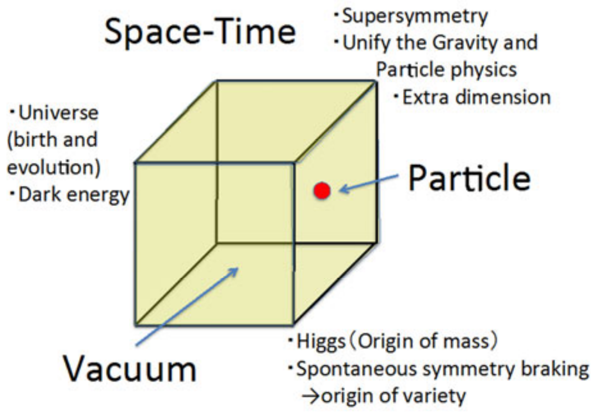
Title of Project : New expansion of particle physics of post-Higgs era by LHC revealing the vacuum and space-time structure

Shoji Asai
(The University of Tokyo, Graduate School of Science, Professor)

Research Project Number : 16H06488 Researcher Number : 60282505

【Purpose of the Research Project】

LHC (Large Hadron Collider) is the energy frontier collider operated at CERN and we have discovered the Higgs boson at LHC, it is the evidence that our vacuum plays important roles for Particle physics and Cosmology. We will discover Supersymmetric particles (or another phenomena beyond the Standard Model) using LHC. Based on these experimental results, we explore researches of the structure of vacuum, the origin of mass, the relation of particle and scape-time. These researches make paradigm-shift including "particle", "vacuum" and "space-time".



【Content of the Research Project】

(1) The Center of Mass Energy of LHC increases upto 13-14TeV. We focus on discovering a new phenomena beyond the Standard Model using LHC. Supersymmetry(SUSY) is the most promising candidate beyond the Standard Model. Studying SUSY particles, we identify "Dark Metter" in the Universe. We extend to study from the Particle physics to Cosmology. Also SUSY is a new symmetry related "Space-Time", and it bridges a missing link between particle and gravity.
(2) Using the Higgs boson, we study detail properties of the Higgs field, which fills in "Vacuum". Phase transitions of our vacuum have driven an evolution of the Universe and changing particle properties.
(3) We study "Space-Time" and "Vacuum" using particles (Higgs boson, SUSY particles and heavy particles such as top quark and W/Z Gauge bosons.)
(4) New technologies of a detector and an accelerator are developed for future experiments, especially for High-Luminosity LHC and FCC.

【Expected Research Achievements and Scientific Significance】

(1) SUSY is the fundamental symmetry to exchange Boson and Fermion. The lightest Supersymmetric particle is a good candidate of the dark matter in the Universe. Furthermore SUSY is the necessary symmetry to unify the general relativity and the quantum theory.
(2) Higgs Boson unifies partially the electromagnetic force and the weak force. SUSY will unify completely three forces, EM, weak and strong forces (Grand Unified Theory).
(3) We determine stability of our vacuum using the Higgs boson. We examine also the detail history, namely Why is our Universe born? How makes evolution? What happen in Future?
(4) Development of the advanced technologies for the detector and accelerator. These will be used in The High Luminosity LHC project and we can expect many spin-off.

【Key Words】

SUSY (SUSY is a symmetry relates to a spin of particle and the most promising theory beyond the Standard model.)

Higgs Field (It gives mass to all particles, and hides in vacuum. The excited state of this field is the Higgs Boson, which is discovered at LHC.)

【Term of Project】 FY2016-2020

【Budget Allocation】 1,017,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.icepp.s.u-tokyo.ac.jp/vacuum-space-time/

Title of Project : Science of Slow Earthquakes

Kazushige Obara
(The University of Tokyo, Earthquake Research Institute, Professor)

Research Project Number : 16H06472 Researcher Number : 40462501

【Purpose of the Research Project】

Our research will shed light on the mystery of "slow earthquakes", which have been detected in succession in recent years. This will require an approach integrating the conventional fields of geophysics, seismology, and geodesy with materials science and non-equilibrium statistical physics, among others. By explaining the mechanisms, environmental conditions and principles of slow earthquakes, our goal is to accelerate a unified understanding of all earthquake events, from low-speed deformation to high-speed slip, and at the same time, to rebuild the way research is conducted on earthquakes.

【Content of the Research Project】

It has been less than 20 years since the discovery of slow earthquakes, and their basic mechanisms are still largely unknown. They occur deep underground, and the materials and physical conditions at that depth are also unknown. Furthermore, the physical laws governing these events clearly differ from those for regular earthquakes, and a qualitative understanding of these events is still sorely lacking. To shed light on such slow earthquakes, we will conduct research in the following areas using a multidisciplinary approach.

- Research topic (A): Explaining the mechanisms involved in the occurrence of slow earthquakes

Using temporal seismic and geodetic observations at inland and offshore areas, and advanced data analysis techniques, we will determine the size and location of slow earthquakes, as well as their spatiotemporal variation, with high precision and high resolution.

- Research topic (B): Explaining the environment in which slow earthquakes occur

By comparing geophysical data obtained from structural explorations with observations based on materials science and rock mechanics experiments, we will reveal the subsurface structure, material composition, and heterogeneity of regions where slow earthquakes occur.

- Research topic (C): Explaining the principles by which slow earthquakes occur

Combining large-scale numerical simulations with basic physical theories and analogue experiments, we will explain physical laws governing slow earthquakes and the physical conditions at their locations.

【Expected Research Achievements and Scientific Significance】

This study will reveal the relationship between slow and huge earthquakes will enable us to provide the basic information for preventing or mitigating disasters via long-term assessment of major earthquake occurrence and other methods. As the occurrence of slow earthquakes is easier to predict than that of regular earthquakes, they are arguably at the frontier of our earthquake prediction ability. Clearly explaining slow earthquakes should serve to broaden our collective knowledge of the possibilities and difficulties of predicting typical earthquakes.
Japan is currently at world-class level in slow earthquake research. Putting our efforts toward reaching the next level will secure our leadership in international research collaboration, and the resulting research network will also be a great benefit to our international contribution by leveraging it for giving recommendations on earthquake disaster prevention policies to other countries at risk of earthquakes.

【Key Words】

Slow earthquake: An earthquake event with a fault rupture that progresses slowly compared to regular earthquakes. Since around the year 2000, various types of slow earthquakes have been found all over the world, mainly in subduction zones.
Subduction zone: Region where an oceanic plate submerges under a continental plate. Huge earthquakes occur at the interface between such plates, while the main regions generating slow earthquakes are the vicinities of huge earthquake seismogenic zones.

【Term of Project】 FY2016-2020

【Budget Allocation】 1,070,800 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.eri.u-tokyo.ac.jp/project/sloweq

Title of Project : Creation of Complex Functional Molecules by Rational Redesign of Biosynthetic Machineries

Ikuro Abe
(The University of Tokyo, Graduate School of Pharmaceutical Sciences, Professor)

Research Project Number : 16H06442 Researcher Number : 40305496

【Purpose of the Research Project】

Natural products have been an important source of medicinal drugs. However, the number of natural products isolated using traditional isolation techniques is declining. Therefore, we need to develop new strategies to obtain new natural products. Recently, genome sequencing data for most living organisms have become available, which enable us to gain instant access to genes encoding biosynthetic enzymes. In addition, with the development of techniques for protein structure analysis, we can better understand the reaction mechanisms and substrate specificities of enzymes. As the tools (genetics and enzymology) and materials (genes and enzymes) are becoming available, natural products scientists are advancing from simply learning biosynthetic machinery to designing new blueprints for producing unnatural compounds. To supply sufficient quantities of the products, it is necessary to design microbial hosts for the expression of the biosynthetic genes. For this purpose, we will construct a new technology platform for the rational redesign of biosynthetic machinery with the help of knowledge and techniques from various research fields including enzymology, organic chemistry, protein, and structural and synthetic biology.

【Content of the Research Project】

In order to achieve our aims, we will set up three intensive research programs (A01-A03).
A01: Creation of Artificial Biosynthetic Machineries. Based on the structural information of enzymes, we will mutate and develop them into new biocatalysts. These biocatalysts will be employed to produce novel compounds using unnatural substrates and/or molecular probes. In addition, we will combine multiple reactions to produce compounds with complex structures.
A02: Construction of Biological Systems for Mass Production. We will establish a methodology to upregulate the production of metabolites whose yield is low in nature. For this purpose, in vivo activation of dormant biosynthetic pathways and heterologous expression will be employed. In order to construct a versatile host for heterologous expression, we will study the crosstalk between the primary and secondary metabolisms by manipulating precursor-supplying pathways in a model microorganism.
A03: Structure and Function of Biosynthetic Enzymes. We will exploit new biosynthetic pathways to find new biocatalysts. We will investigate in detail the reaction mechanisms of the focused enzymes using X-ray crystallography. Evolutionary analysis of biosynthetic genes and a genome editing method will also be employed in this investigation.

【Expected Research Achievements and Scientific Significance】

Enzymes are excellent at producing optically-active compounds. Their abilities to produce complex chemical structures are astonishing. Compared to chemical synthesis, enzymatic synthesis is more ecologically friendly, since it does not need an organic solvent. The disadvantages of enzymes are their high-substrate specificity and the difficulty of controlling their reaction mechanisms. Nowadays, these disadvantages may be overcome by understanding their catalytic mechanisms. In this project, we will establish a methodology to engineer the catalytic activity of enzymes to produce desired compounds, and utilize the resultant catalysts to produce compounds with an industrial-level yield. These achievements will pave a way to construct artificial biosynthetic pathways to produce supra natural products.

【Key Words】

Engineered Biosynthesis; Synthetic Biology, Natural Products; Enzyme; Gene; Enzyme Engineering; Metabolic Engineering; Biocatalysis.

【Term of Project】 FY2016-2020

【Budget Allocation】 1,106,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.f.u-tokyo.ac.jp/~tennen/bs_index-e.html

Title of Project : Nano-Material Manipulation and Structural Order Control with Optical Forces

Hajime Ishihara
(Osaka Prefecture University, Graduate School of Engineering, Professor)

Research Project Number : 16H06503 Researcher Number : 60273611

【Purpose of the Research Project】

This project aims at the realization of optical force technologies for mechanical manipulation (trapping, transportation, positioning, and aligning) of individual nano-objects, such as molecules and quantum dots, in a direct and selective way according to their individual properties, leading to scientific principles of a novel scheme for creating structural order through the manipulation of microscopic substances. To achieve the technologies of manipulating the mechanical motion of individual nano-objects, we develop the design method for optical forces using linear and nonlinear optical responses of various targets exhibiting quantum mechanical properties. Our project will realize novel schemes to create structural order reached only by optical force technologies, e.g., optical sorting and isolation of targets in different quantum resonance conditions, manipulation of crystal morphology and alignment, and manipulation of chemical processes by selective control of molecular diffusion and condensation.

【Content of the Research Project】

To visualize the achievement of our goal, we will conduct the following three collaborative subprojects: [A] Isolation of particular kinds of nano-objects and their precision arrangement over a macroscopic region, [B] control of interparticle interactions for the creation of hierarchical structures including crystallizations, and [C] control of chemical processes through selective manipulation of molecules. Furthermore, we set four planned researches that are the bases of the above subprojects, i.e., A01: Theories, metrologies, and observations of optical forces for establishing basics of optical manipulation (“basics of optical forces”), A02: advancement of manipulation methods utilizing the microscopic degrees of freedom of matter systems (“creation of optical forces”), A03: single molecular manipulation on the nanometer scale by utilizing localized electric field, and the operation over macroscopic regions (“ultimate scheme of optical forces”), and A04: creation of superstructures and new phenomena by selective control of interparticle interactions (“exploitation of optical forces”). We will achieve these three subprojects by synergizing the four planned researches.

Because researchers from a variety of fields such as physics, chemistry, and engineering join this project, we manage several “training dojos” where young researchers can learn methods of different fields, which will strongly promote collaboration for the subprojects [A], [B], and [C], and build the ability of young researchers.

【Expected Research Achievements and Scientific Significance】

Scientific principles and technologies realized by this project will lead to the following achievements. (1) Selective motion-control and observation of spatial arrangement of nano-objects on the molecular scale enable technologies for unconventional metrology, screening, and visualization that cannot be performed using existing methods. (2) Control of interparticle interactions by manipulating the local density and orientation of particles in high-concentration solution enables novel design of crystallization and self-assembly of nanoparticles. (3) Manipulation of local diffusion and density of particular kinds of particles using optical forces enables unconventional schemes for studying and controlling chemical processes, novel types of position-selective molecular sensing, and technologies to dramatically improve efficiencies of chemical reactions.

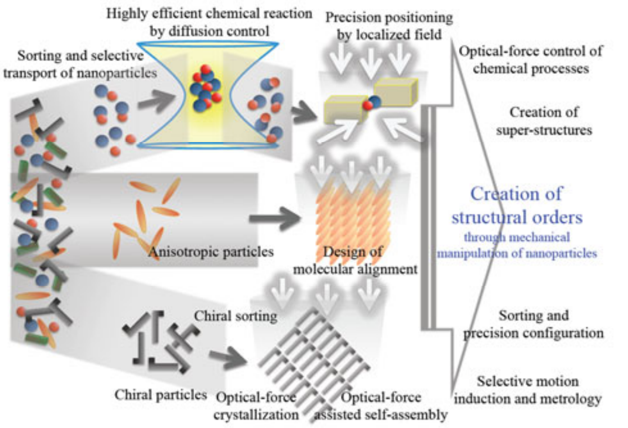


Figure: Schematic image of structural order control using optical manipulation of nanoparticles

【Keywords】

Optical force: A force arising from either momentum transfer when light is scattered and/or absorbed by a matter system or the electromagnetic interaction between the applied field and the induced polarization.

Localized electric field: Oscillating electric field associated with localized plasmons sustained in metallic nano/microstructures, usually enhanced by several orders of magnitude compared with the incident field intensity.

【Term of Project】 FY2016-2020

【Budget Allocation】 1,049,900 Thousand Yen

【Homepage Address and Other Contact Information】
http://optical-manipulation.jp

Title of Project : Synthesis of Mixed Anion Compounds toward Novel Functionalities

Hiroshi Kageyama
(Kyoto University, Graduate School of Engineering, Professor)

Research Project Number : 16H06438 Researcher Number : 40302640

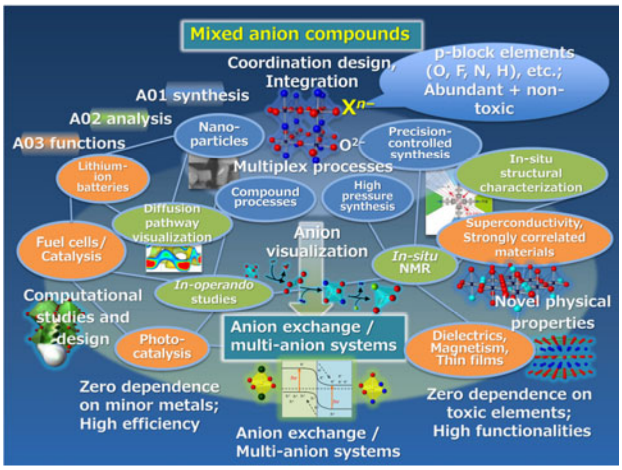
【Purpose of the Research Project】

Given the scarcity of resources for our nation, keeping a technological advantage is vital for preserving our industry's competitiveness as a whole. We believe the development of new materials is necessary for this. Recently, mixed anion compounds consisting of multiple anions within a single compound have gathered attention. The use of multiple anions enables unusual coordination modes and crystal structures, giving them a huge potential for new properties when compared to existing oxides or nitrides. While mixed anion compounds will occupy a central stage in materials development, the field is still quite new. In this project we will establish the scientific foundations of mixed anion chemistry, establish Japan's pre-eminent position in the field, and contribute to industry by providing new mixed anion materials.

【Content of the Research Project】

The scientific community in materials science is divided into many narrow disciplines. This project will unite the community and field using mixed anion systems as a rallying point. We envision a multidisciplinary team working together to develop new mixed anion compounds and explore their functions. Our team will be divided into subgroups addressing the synthesis, analysis, and functional properties of mixed anion compounds, based on these key components of the materials discovery cycle. These subgroups will work together to solve problems difficult to address with conventional non-mixed anion systems. Our multidisciplinary approach will also be invaluable in training new scientists for the next generation.

The synthesis subgroup (A01) will focus on the discovery of new mixed anion compounds based on various synthesis techniques. The group's efforts will involve complex reactions, establishing the principles controlling crystal structure, and use computational techniques for material design. The analysis group (A02) will use various diffraction and spectroscopy techniques to solve various characterization issues inherent to mixed anion systems. Combining these results with insight obtained from *ab initio* calculations will enhance our understanding of the materials' physical properties. The functions subgroup (A03) will channel these materials to provide solutions for various energy-related applications. The subgroup will make various connections between function and crystal/electronic structure, providing feedback to the further synthesis of new mixed anion compounds.



【Expected Research Achievements and Scientific Significance】

Mixed anion materials differ greatly from conventional materials, making radically new functions and applications possible. Additionally mixed anion systems focus on the effects of elements such as hydrogen, chlorine, phosphorus, carbon, etc. (in anionic form). As these elements are quite ubiquitous, our approach to materials development is relatively unimpeded by conventional problems of resource scarcity and distribution.

Until now, individuals separated by various fields and applications have led materials development. In this project, young scientists will be trained without such conventional barriers between fields. While training the next generation of scientists, we will contribute to raising the overall level of our nation's academic and technological prowess.

【Key Words】

Mixed anion compounds, ubiquitous elements, crystal chemistry, crystal engineering, analytical techniques, synchrotron radiation, theoretical calculations, electronic structure, local structure, chemical bonding, fuel cells, catalysis, rechargeable batteries, photocatalysis, photoelectrochemistry, dielectrics, fluorescent materials, magnetic materials, thermoelectrics, superconductors.

【Term of Project】 FY2016-2020

【Budget Allocation】 1,022,800 Thousand Yen

【Homepage Address and Other Contact Information】

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