Title of Project： Physical Properties of Quantum Liquid Crystals

SHIBAUCHI Takasada
(The University of Tokyo, Graduate School of Frontier Sciences, Professor)

Research Project Number：19H05822 Researcher Number：00251356

【Purpose of the Research Project】

In rod- or disk-shaped molecular systems, a state called "liquid crystal" appears in addition to the three states of matter; gas, liquid, and solid. Recently, electronic states that have similarities to liquid crystals have been observed in a variety of solid materials. These electronic states have been studied independently in the fields of quantum spins, strongly-correlated metals, and superconductivity, but here we define these states respectively as "spin liquid crystals", "charge liquid crystals" and "pair liquid crystals". In this innovative area research, we introduce a new concept "quantum liquid crystals" (QLCs) to unify these novel electronic states.

Within this, we will promote new collaborations between researchers from different fields, to clarify and control the physical properties of QLCs. We aim to understand the ground states of different QLCs; to establish the universal features common to all QLCs; and to understand the diversity of phenomena seen in experiment. In addition, by using state-of-the-art technologies, we will elucidate and control the elementary excitations of QLCs. This will lay the foundation for future QLC-based technologies exploiting the flexible characteristics of liquid crystals, and the large and fast responses of quantum systems.

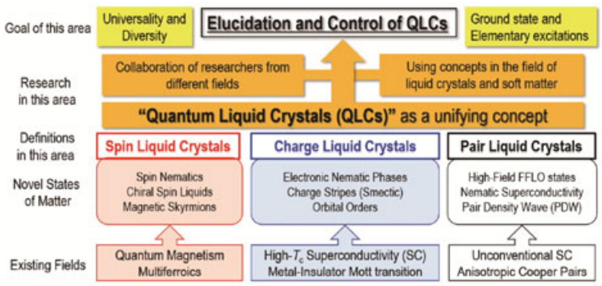

Figure1. Outline of the research project

【Content of the Research Project】

Within this innovative research area, we have identified four different themes, based on methodology, which will be used to promote new collaborations.

-A01: Development of QLC materials

To develop and characterize new materials in which novel QLC states emerge, using a broad range of established and original synthesis techniques.

-B01: Advanced measurements of QLCs

To elucidate QLC electronic states in experiment, by using a combination of established high-precision measurement techniques and through the development of new techniques, in combination with different technologies.

-C01: Theory of QLCs

To describe the order parameters of QLCs and effects of their quantum fluctuations, as well as to design QLC materials and their functionality.

-D01: Control and functionality of QLCs

To control QLC states and search for useful QLC functions, by utilizing micromachining-based nanoscience and ultrafast optics.

Research in this area will be interdisciplinary, and aims to establish the basics of new quantum technologies.

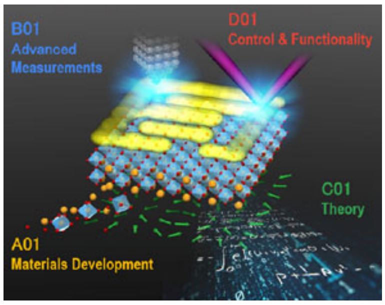

Figure2. Four themes to study QLCs

【Expected Research Achievements and Scientific Significance】

The advances in the field of "liquid crystals and soft matter" beyond the three states of matter have successfully led to many technological applications. Our QLC area can be considered as its quantum version, which can potentially generate novel phenomena and concepts. It will also pave a pathway to new QLC technology that has some useful functions in the quantum information.

【Key Words】

Quantum liquid crystals (QLCs): New electronic states similar to liquid crystals emerging from quantum effects. In liquid crystals molecules have anisotropy, but in QLCs quantum-mechanical degrees of freedom lead to anisotropic states with peculiar physical properties.

【Term of Project】FY2019-2023

【Budget Allocation】1,134,000 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Mid-latitude ocean-atmosphere interaction hotspots under the changing climate

NONAKA Masami
(Japan Agency for Marine-Earth Science and Technology, Application Laboratory, Group leader)

Research Project Number : 19H05695 Researcher Number : 90358771

【Purpose of the Research Project】

Frequency of extreme rainfalls and snowfalls has been increasing these years, and those events severely affect human lives and properties.

It has been considered that tropical ocean and atmosphere variability such as El Niño, as well as the warming climate, remotely influences mid-latitude extreme weather/climate, while the mid-latitude ocean is passive to atmospheric variability. Current operational seasonal climate predictions are conducted based on this climate “assumption.”

Recent high-resolution ocean/atmospheric data analyses, however, have revealed that mid-latitude ocean also influences atmospheric circulations and their variability. Rediscovering strong warm current (e.g., the Kuroshio and the Gulf Stream) and associated strong ocean frontal zones as “*climate hotspot*”, we have elucidated mechanisms of ocean-atmosphere interactions and established a new paradigm of active roles of mid-latitude oceans in the climate system, replacing the conventional “assumption.”

The research progress has prompted a new crucial task: application of such new knowledge to predictions of extreme rainfalls/snowfalls and climate variability. In the present project, I) we will further our understandings of mid-latitude ocean-atmosphere interaction processes that span multiple spatio-temporal scales and interplay among them through tight collaborations of latest observational and numerical modeling tools. Also, based on the improved understandings, II) we investigate predictability of extreme weather (such as typhoons and bomb cyclones), of persistent atmospheric circulation anomalies that induce those extremes, projection of climate changes, and active roles of mid-latitude oceans in those phenomena. The purposes of the present project are then deepening of the previously established paradigm and showing its scientific and societal importance and validity.

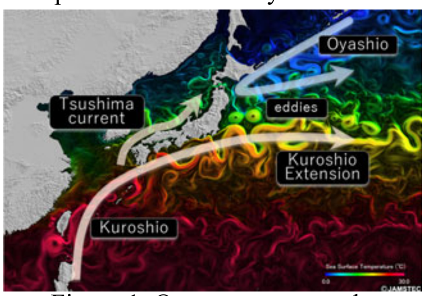

Figure 1. Ocean currents and temperature around Japan

【Content of the Research Project】

For I), we conduct an intensive observational campaign of both atmosphere and ocean in the Tsushima warm current region located upwind of Japan with directly impacts on its climate, utilizing state-of-the-art observational equipment. We further expand our understanding of ocean-atmosphere interactions with their linkage to atmospheric substances through investigations of impacts of heat and aerosols exchanges between ocean and atmosphere on low-level clouds and marine ecosystems.

For II), our studies will extend to evaluations of potential improvements of prediction and/or uncertainty of disaster inducing atmospheric circulation anomalies and extreme rainfall/snowfall, by considering active influences from mid-latitude oceans. Also, we will try to obtain general understandings of roles of *climate hotspot* under the changing climate and its impacts on uncertainty of climate change projection.

【Expected Research Achievements and Scientific Significance】

Three achievements are expected: 1. Further deepening of our understandings of multi-scale ocean-atmosphere interactions and their mechanisms. 2. Evaluations of possible contributions of ocean-atmosphere interactions in *climate hotspot* and especially ocean’s active roles onto improvements of predictability of extreme rainfall/snowfall, extreme weather events such as typhoon and bomb cyclones, and persistent atmospheric circulation anomalies associated with extreme climate. Also, estimations of predictability of ocean currents and eddies, which induce ocean temperature variability. 3. Basic and general knowledge on overlooked roles of mid-latitude air-sea interactions for the warming climate. This will make the first estimation of uncertainty of climate change projection caused by mid-latitude ocean-atmosphere interactions in climate projection models. Through these developments in the fields of *predictability* and *global warming*, wide societal impacts are expected from the present project.

【Key Words】

mid-latitude air-sea interactions (ocean and atmospheric affect each other to induce their structure and variability)
extreme weather/climate (unusual state such as extreme rainfalls and snowfalls with several days scale, and such as cool summer and warm winter with seasonal scale)

【Term of Project】 FY2019-2023

【Budget Allocation】 1,138,000 Thousand Yen

【Homepage Address and Other Contact Information】

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Science and Engineering

Title of Project : New Materials Science on Nanoscale Structures and Functions of Crystal Defect Cores

MATSUNAGA Katsuyuki
(Nagoya University, Graduate School of Engineering, Professor)

Research Project Number : 19H05785 Researcher Number : 20334310

【Purpose of the Research Project】

In this project, specific electronic and atomic structures of grain boundaries, interfaces and dislocations that can realize novel and distinct materials properties are defined and referred to as "crystal defect cores". Researchers specializing in theoretical calculations, nanoscale characterization and advanced materials processing conduct collaborative studies, aiming at creating a new area in materials science named "crystal defect core". Through establishing new scientific principles based on the concepts of "crystal defect core", we will further explore novel properties and materials due to crystal defects.

Conventional studies have focused on average bulk structures and macroscopic properties of materials in general, and thus understanding of crystal defects is often limited to their static and averaged atomic pictures. Recent technological progresses in methods and approaches of nanoscale characterization and computational science are so remarkable that we have been enabled to acquire quantitative information on nanoscale structures of crystal defects. These advanced approaches and methods have facilitated our more in-depth understanding about the crucial roles that the crystal defects play for realizing various materials properties. For future materials design and development, it is essential to reveal relationships between nanoscale structures of crystal defects and materials properties. Thus, in this project, we aim at discovering or creating new materials functions and new exploratory materials based on "crystal defect cores", including those emerging under external stimulus including thermal, electric, magnetic, optical or stress fields.

【Content of the Research Project】

This research project has three major Research items as follows:

A01: Modeling and design of crystal defect cores
A02: Nanoscale characterization of crystal defect cores
A03: Materials development based on crystal defect cores

In Research items A01 and A02, we focus on basic science of crystal defects. We do collaborative and systematic researches of grain boundaries, interfaces and dislocations so as to establish new scientific principles based on in-depth understanding of a structure-property relationship of the crystal defects, by means of theoretical calculations, materials informatics and nanoscale characterization at the world-class highest level. Researches in the Research item A03 of materials processing come from diverse materials fields, and try to develop novel materials and their properties by controlling crystal defects at the nanometer scale. Throughout the research area, it is expected for our intensive and extensive collaborations to prove that "crystal defect core" is a universal concept to realize novel materials development in the next generation.

【Expected Research Achievements and Scientific Significance】

■ To establish new scientific principles to make it possible to explore novel and distinct materials properties originating from crystal defects

■ To discover or create new materials with remarkable properties in diverse fields of materials science

■ To facilitate considerable technical development of theoretical calculations, nanoscale characterization, and materials processing.

Our concept of "crystal defect core" will provide a scientific impact when we succeed in developing materials and their properties through precisely controlling crystal defect cores. This is because crystal defects have been thought to play a negative role for materials properties. This research area can find out a new strategy for controlling crystal defect cores so that they play positive roles for better properties, paving a new avenue for future materials developments.

【Key Words】

Crystal defects: Irregular atomic arrangements in crystalline materials.

Crystal defect cores: Specific electronic and atomic structures that can realize novel and distinct materials properties

【Term of Project】 FY2019-2023

【Budget Allocation】 1,098,000 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Aquatic Functional Materials: Creation of New Materials Science for Environment-Friendly and Active Functions

KATO Takashi
(The University of Tokyo, Graduate School of Engineering, Professor)

Research Project Number : 19H05714 Researcher Number : 70214377

【Purpose of the Research Project】

In this project, Aquatic Functional Materials is defined as materials that harmonize and interact with environment and bio-systems in the existence of water. The objective of this project is to create and establish materials science on Aquatic Functional Materials and to develop innovative materials by fusion of materials science and basic science of water. Water is essential for the sustainable development of human civilization as described in the SDG6 of the United Nations. It is our emergent issues to develop Aquatic Functional Materials serving in a wide range of the fields including environment, energy, healthcare and agriculture.

【Content of the Research Project】

The specific feature of our project is to understand the interactions between water and materials in the level of molecules and molecular nano-assemblies based on fundamental science of structure-function relationship between water and materials for the creative development of Aquatic Functional Materials. We study on Aquatic Functional Materials from a wide range of standpoint of views including organic chemistry, polymer chemistry, experimental physics, computational science, and engineering.

As bio-system and global environment do not function without water, we focus on behavior of water as molecules for materials science. In this project, we define aquatic environments as living and industrial regions where water exists, and bio-system as well as hydrosphere because there are common features that interactions of water molecules with molecules and materials play key roles.

New principles of materials design are required to develop materials that exhibit high function in aquatic environments. We need to establish unified materials science based on understanding of structure-function relationship between water and substance. In conventional water science, structures and properties of water as single components have been mainly studied. In conventional materials science, for example, electronic materials and polymer materials to be used in non-aquatic circumstances have been intensively focused. It is our intention that we unify science of water and materials science together and further develop to establish science of Aquatic Functional Materials.

Figure 1. Fusion of sciences and engineering for the achievement of research in this project.

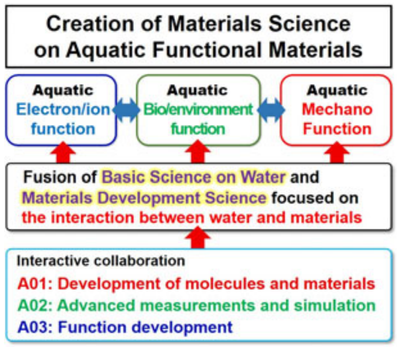

Figure 2. Scheme of research in this project.

【Expected Research Achievements and Scientific Significance】

1. Creative development of innovative materials that function in aquatic environments

The development of highly functional materials in the coexistence with water, which were not well studied, is expected. For example, we expect the fabrication of aquatic electron/ion functional materials

2. Creation of Science of Aquatic Functional Materials

New science that gives design principles for materials that exhibit high functions in aquatic environments will be established by fusion of basic science of water and materials science.

【Key Words】

Aquatic Functional Materials: In this project, materials that function in the living and industrial regions where water co-exists, and bio-system as well as hydro-regions of ocean and river of sphere are defined as Aquatic Functional Materials. It is because that when we examine behavior of water and interactions of water in molecular level, there are common issues in science.

【Term of Project】 FY2019-2023

【Budget Allocation】 1,185,200 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Unraveling the History of the Universe and Matter Evolution with Underground Physics

INOUE Kunio
(Tohoku University, Research Center for Neutrino Science, Professor)

Research Project Number : 19H05802 Researcher Number : 10242166

【Purpose of the Research Project】

We aim at unraveling the history of the universe and matter evolution to answer “How is matter created?”, “How are galaxies/stars formed?”, “How are elements created?” and “How do they end up with the earth?”, by concentrating all efforts of underground astroparticle experiments covering neutrino-less double beta decay ($0\nu2\beta$), dark matter (DM), supernova (SN) and geo-neutrino (ν). The vigorous cooperation at “Kamioka” will expands to world-wide, and newly involved subjects (low temp. sensors, nuclear matrix element, DM distribution, SN explosion and matter evolution theory) will further deepen each research field and enhance the synergy among them. It will sustain the competitiveness and superiority in the world and contribute to nurture young talents.

【Content of the Research Project】

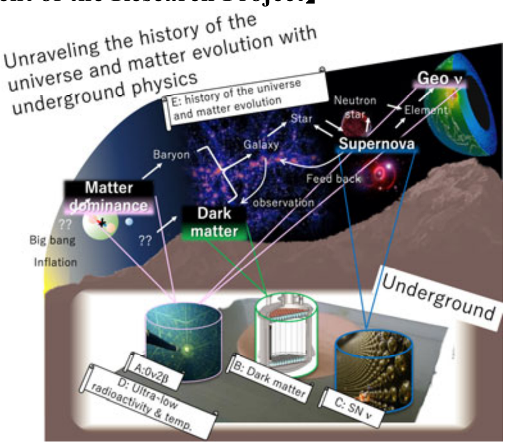

Figure1. Research projects and relevant subjects

KamLAND-Zen is leading the search for $0\nu2\beta$ in the world. XENON has been leading the direct search of DM and is evolving to XENONnT. Super-Kamiokande has the world best sensitivity on SN-ν detection and is upgrading to SK-Gd. KamLAND is the pioneer of and leading geo-ν observation. We develop the cooperation among these top-runners and challenging projects for future on the common technologies. As challenging projects, a $0\nu2\beta$ experiment involves isotopic enrichment and scintillating bolometer aiming at an ultimate sensitivity, and directional detection of DM develops under the world cooperation to overcome the limit of neutrino floor. The ultra-low radioactivity technology as the common base will pursue the world-best performance and raise the technological floor of the whole field sharing and internationalizing the low-BG database. We also incorporate low-temp. sensors as novel techniques to improve energy resolution and to achieve lower threshold for new science frontiers, and sustain the competitiveness. Moreover, we aim at a seamless connection of particle cosmology and matter evolution picture as a theoretical flamework that spans the history of the universe from the beginning to the present. It will largely enhance the synergy of research in this area and the connection to diverse fields.

【Expected Research Achievements and Scientific Significance】

We propel researches on the most important subjects in underground astroparticle physics, search for $0\nu2\beta$ and direct detection of DM, and also SN relic ν and geo-ν detection those provide important information of matter evolution in the universe. These top-runners are closest to world’s first big discoveries. Developing the common novel technologies and theoretical flamework of the whole history of the universe will inspire surrounding fields, therefore, this area continues to be a core of the field of underground astroparticle physics. The international cooperative environment we realize will largely contribute to nurture young active talents in the world.

【Key Words】

Underground astroparticle physics: experimental researches of rare phenomena connected with particle, nuclear, cosmological, astronomical and geo- science run at underground ultra-low radioactivity environment
Neutrino-less double beta decay ($0\nu2\beta$): unique realistic phenomenon to verify the ν/anti-ν identity as a key to explain the matter dominance in the universe
Dark matter (DM): Yet undiscovered elementary particle indispensable for the structure formation of the universe, with the halo density around the earth at ~0.3GeV/cm^3
Supernova relic ν: ν cumulatively arriving from past SN explosions that provide information on star formation history, SN explosion mechanism and matter evolution

【Term of Project】FY2019-2023

【Budget Allocation】1,129,500 Thousand Yen

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【Grant-in-Aid for Scientific Research on Innovative Areas (Research in a proposed research area)】

Science and Engineering

Title of Project : Hypermaterials: Innovation of materials science in hyper space

TAMURA Ryuji
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Research Project Number : 19H05817　Researcher Number : 50307708

【Purpose of the Research Project】

The discovery of quasicrystals, with high symmetry impossible for three-dimensional periodic crystals, has brought about a paradigm shift in crystallography and has overturned the definition of crystals that have been accepted for hundreds of years. The quasicrystal has a cross-sectional structure of a high-dimensional periodic crystal, and another extra space called "complementary space" is required to describe the atomic structure. This project aims at establishing a new concept of substances, "hypermaterial", which is a high-level concept that includes the existing concept for substances, and also at creating a new theory that incorporates the concept of hypermaterial.

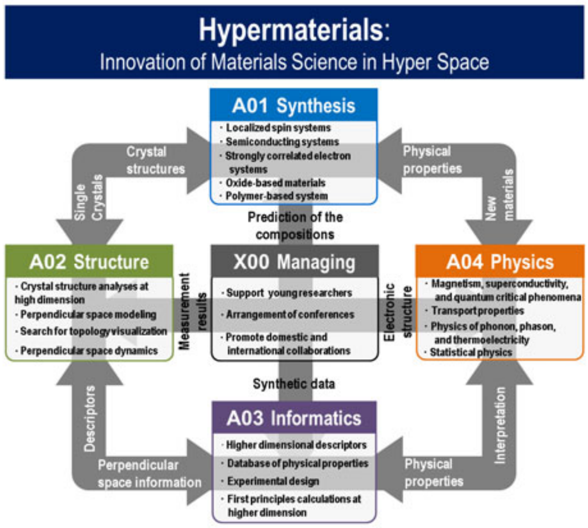
【Content of the Research Project】

In order to achieve the above purpose, this project will be conducted with four research groups (Figure).

[A01] Synthesis of Hypermaterials
[A02] Structure of Hypermaterials
[A03] Hypermaterials Informatics and the Search for Hidden Orders
[A04] Physics of Hypermaterials and the Search for Hidden Orders

The A01 group challenges to synthesize new metallic, semiconducting, ceramic, and polymer hypermaterials, partly based on the material compositions provided by the A03 group. In the A02 group, the static and dynamic structure of the newly synthesized hypermaterials are investigated by using X-ray, neutron beam, etc. In the A03 group, a database of hypermaterials is constructed, and the descriptors related to the stability of hypermaterials will be identified. Also, the descriptors related to the structure and physical properties of hypermaterials are searched in the real space as well as in the complementary space, and predictions of the compositions and physical properties of hypermaterials are performed. In the A04 group, the physical properties of the newly synthesized hypermaterials are measured, and the states of electrons, spins, phonons, etc. are investigated. Also, in cooperation with the A02 group, the physical quantities are mapped to the complementary space in order to elucidate the hidden orders, and their interpretation is performed.

Through active collaborative research among the four research groups, we will search for new physical properties and new phenomena, which cannot be obtained with conventional crystals, and will create new materials science based on the complementary space.



Organization of the Project

【Expected Research Achievements and Scientific Significance】

1. Hidden orders behind the complex behaviors of hypermaterials will be elucidated, and a new theory that incorporates the hidden orders will be developed.
2. The hypermaterial is a high-level concept of substances including existing periodic crystals, and this project will bring us a new material view, that is, leading us to view the structural information in the complementary space.
3. The world of hypermaterials will expand not only in metals, but also to semiconductors, ceramics, polymers.

【Key Words】

Hypermaterial: Abbreviation of "material" in "hyper space (high-dimensional space)". Quasicrystals and approximant crystals can be described as cross-sectional structures of high-dimensional periodic crystals. Hypermaterials refer to the substances described in a high-dimensional space in a unified way, and are characterized by having structural information not only in the real space but also in the "complementary space".

【Term of Project】 FY2019-2023

【Budget Allocation】 791,200 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.rs.tus.ac.jp/hypermaterials/html

Science and Engineering

Title of Project : Science on Interfacial Ion Dynamics for Solid State Ionics Devices

IRIYAMA Yasutoshi
(Nagoya University, Graduate School of Engineering, Professor)

Research Project Number : 19H05812　Researcher Number : 30335195

【Purpose of the Research Project】

Solid-solid interfaces generate entirely new functions different from the intrinsic nature of each solid material. In this project, unique interfacial ion dynamics around the hetero/homo interfaces of solid state ionics materials (SSIM) are systematically investigated so as to establish design principles for fast ion transport and concentrated ion storage around interfaces, that is, "*Interface Ionics*".

【Content of the Research Project】

There are two kinds of SSIM; i) insertion electrode material (electrode), where electrons or holes move faster than ions. ii) solid electrolyte, where ions moves faster than electrons or holes. When these two SSIMs are combined, an equilibrium state is formed through the rearrangement of all the charged carriers (electron, hole, and ion) and then their electrochemical potentials become equal. As a consequence, the electrode/solid electrolyte interface obtains different properties with each intrinsic SSIM due to space charge layer formation, mechanical relaxation (strain distribution), etc., which provide unique interfacial ion dynamics (Fig. 1). The aim of this project is to investigate these physical and chemical modulations around the interface in detail and establish the interface design principle which makes it possible to generate novel functions around the interfaces. This project integrates chemistry, physics, advanced measurement, theory and data science, and material science and consists of the four research groups (Fig. 2).

Gp-A01 fabricates model interfaces using single

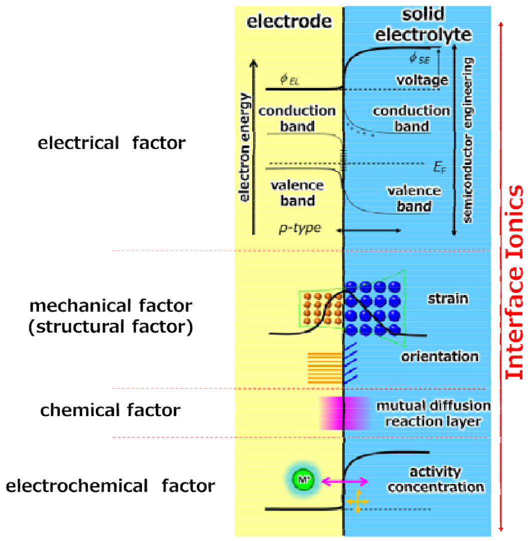


Fig.1 Schematic image of various factors affecting "*Interface Ionics*".

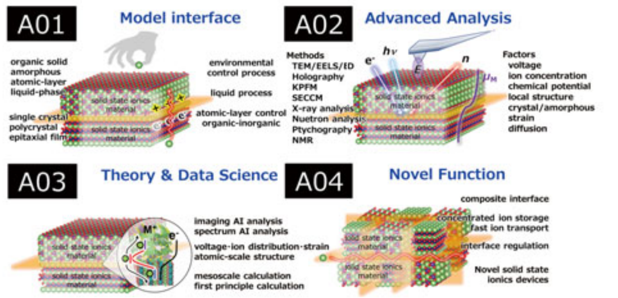


Fig. 2 Overview of research groups.

crystalline substrates, epitaxial thin films, etc. and investigates their interfacial ion dynamics. Gp-A02 analyzes modulation and distribution of voltage, ion concentration, chemical potential, local structure, etc. around the interface using advanced measurements. Gp-A03 clarifies ions and electrons distribution and their dynamics around the interface using multi-scale theoretical calculation and informatics analyses. Gp-A04 develops advanced materials especially focusing on metastable phases with lattice defects and lattice strains by combining crystalline and amorphous SSIMs.

【Expected Research Achievements and Scientific Significance】

"Interface Ionics" clarifies design principle of interface in all-solid-state batteries where fast ion transport and concentrated ion storage is expected in the right space for high-rate charge-discharge reactions and high capacity electrode materials. Furthermore, those interfaces are effective to develop novel solid state ionics devices such as all-solid-state capacitor, superconductor, transistor, actuator, electret, et al.

【Key Words】

Solid State Ionics Devices; Advanced devices using SSIMs such as all-solid-state battery, all-solid-state capacitor, etc.

Interfacial Ion Dynamics; Unique ion dynamics generating around the hetero/homo interfaces of SSIMs.

【Term of Project】 FY2019-2023

【Budget Allocation】 1,127,800 Thousand Yen

【Homepage Address and Other Contact Information】

https://www.interface-ionics.jp/