



Title of Project : HYDROGENOMICS: Creation of Innovative Materials, Devices, and Reaction Processes using Higher-Order Hydrogen Functions

Shin-ichi Orimo
 (Tohoku University, WPI-AIMR, Professor)

Research Project Number : 18H05512 Researcher Number : 40284129

【Purpose of the Research Project】

Hydrogen in materials exhibits a wide range of concentration, high mobility, quantum nature, and superior chemical reactivity. All these features of hydrogen originate from its bonding and size flexibilities. (Fig. 1)

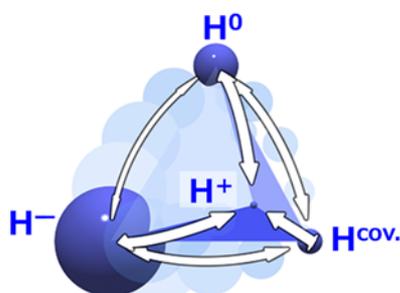


Fig. 1 Hydrogen diagram illustrating the bonding and size flexibility of hydrogen in materials; the spheres located at each vertex represent proton (H⁺), hydride ion (H⁻), covalently bonded hydrogen (H^{cov.}) and neutral hydrogen (H⁰). The sizes of hydrogen are also drastically changed according to the bonding states.

The purpose of this project is to develop a new materials science of hydrogen / hydrides (hereafter referred to as “Hydrogenomics”, i.e., hydrogen-omics) as a guideline to “fully utilize” the diverse functionalities of hydrogen in materials.

【Content of the Research Project】

The project will focus on the four most important functionalities of hydrogen originated from its bonding and size flexibilities (hereafter, referred to as “hydrogen functions”); i.e., “high densification ability (A01)”, “interfacial localizability (A02)”, “fast migration ability (A03)” and “high activation ability (A04)”. Then the project will merge them to induce unprecedented “higher-order hydrogen functions (synergistic effect between its individual hydrogen functions)” with the support of “advanced analysis and simulation techniques (A05)”, which will also be developed within this project to capture the hydrogen functions more accurately than ever done before. (Fig. 2)

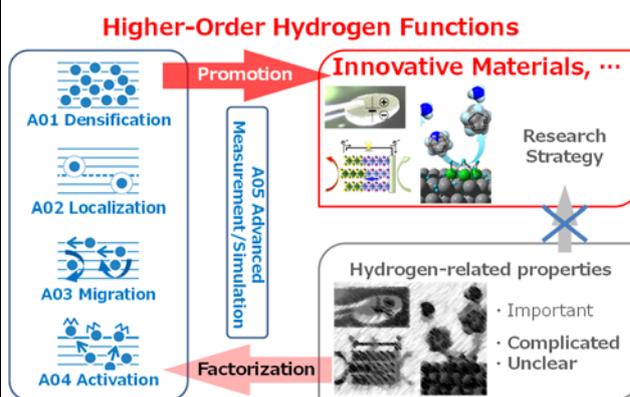


Fig. 2 Strategy of Hydrogenomics.

【Expected Research Achievements and Scientific Significance】

- Synthesis of hydride superconductors and super-ionic conductors.
- Proof-of-principle for hydride electronics, and enhancement of photovoltaics and high-strength steel properties.
- Production of advanced energy generation / storage and new-concept devices using hydrogen-electron coupling and hydride super-ionic conductors.
- Performing new material-conversion processes using hydrogen.
- Clarification of the mechanism determining the hydrogen functions and realization of high-accuracy analysis based on hydrogen data-assimilation technique.
- Promotion of young researchers training and social implementation, and formation of international network, in the related research field.

【Key Words】

Hydrogenomics, Higher-order hydrogen functions

【Term of Project】 FY2018-2022

【Budget Allocation】 1,135,000 Thousand Yen

【Homepage Address and Other Contact Information】

<https://www.hydrogenomics.jp>
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Grant-in-Aid for Scientific Research on Innovative Areas
 (Research in a proposed research area)



Title of Project : A Paradigm Shift by a New Integrated Theory of Star Formation: Expanding Frontier of Habitable Planetary Systems in Our Galaxy

Shu-ichiro Inutsuka
(Nagoya University, Department of Physics, Professor)

Research Project Number : 18H05436 Researcher Number : 80270453

[Purpose of the Research Project]

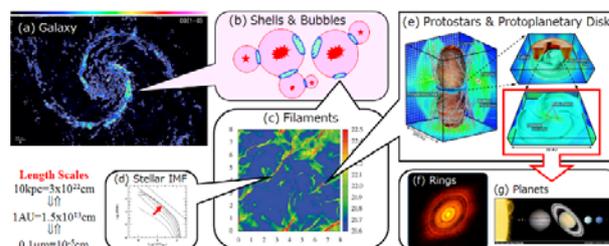
Stars are continuously created in our Milky Way Galaxy. Heavy atomic elements, such as metals, are created inside stars and blown out into the interstellar space of the Galaxy. This process provides atomic elements heavier than hydrogen and helium, such as carbon and oxygen, which is critically important for the existence of living creatures in the universe. In our Milky Way Galaxy, the enrichment of heavy elements starts in the inner Galactic regions and gradually expands toward the outer regions of the Galactic disk. This implies that the environment for creating habitable planets and biological entities are developed inside-out in the Galactic Disk over a timescale of the age of the universe. Understanding the origin and evolution of our solar system requires the comprehension of the environment of the birth place of the solar system about 4.6 billion years ago that is expected to be different from its current location in the Galaxy. This requires our understanding of the evolution of our Galaxy itself, over the timescale comparable to the age of the universe. We will try to understand this by extending the recently developed theory of star formation and describing the formation of star clusters. In addition, we will develop the planet formation theory and try to solve multiple puzzling questions regarding the origin of the solar system. This would be done by the collaboration of all the relevant researchers in Japan and this work is expected to lead a paradigm shift in the investigation of the origin of our solar system. We will also try to find possible siblings of the Sun that would have been born at the same time in the same star cluster, i.e., the expected birth place of the Sun. The results of our project are expected to provide a quantitative picture for the distribution of habitable planets in the Galaxy, and hence, provide a new strategy for future observations of exo-planets.

[Content of the Research Project]

- [A01] Theory for the Formation of Star Clusters and the Evolution of Our Galaxy
- [A02] Theory for the Formation of Planetary Systems from Diverse Protoplanetary Disks
- [A03] Theoretical and Observational Studies of the Formation and Evolution of Diverse

Planetary Atmospheres

- [B01] Observational Studies on the Formation of Star Clusters in Giant Molecular Clouds
- [B02] Observational Studies on the Evolution of Protoplanetary Disks in Diverse Environments
- [B03] Innovation of Infrared Observations of Young Planets and Habitable Planets



[Expected Research Achievements and Scientific Significance]

We will describe the time evolution of the formation rate and the mass function of star clusters and establish a quantitative picture of the Galactic chemical evolution. We will also investigate theoretically and observationally the existence of different types of exo-planets and understand the diversity of planet formation in our evolving Galaxy. These studies are expected to provide a deep understanding on the origin of our solar system.

[Key Words]

Galactic Chemical Evolution: The enrichment of heavy elements in the Galaxy.

Molecular Clouds: Low temperature (~10K) clouds in the interstellar space that are mostly composed of molecular hydrogen: The birthplace of stars.

Protoplanetary Disks: Rotating gaseous disks created around new-born stars: The birthplace of planets.

Exo-Planets: Planetary systems found outside of our solar system.

Habitable Planets: A certain type of planets that may possess liquid water on their surface, and hence, may potentially provide a chance to host biological entities.

[Term of Project] FY2018-2022

[Budget Allocation] 1,109,800 Thousand Yen

[Homepage Address and Other Contact Information]

<http://www.ta.phys.nagoya-u.ac.jp/star/>



**Title of Project : Exploration of Particle Physics and Cosmology
with Neutrinos**

Tsuyoshi Nakaya
(Kyoto University, Graduate School of Science, Professor)

Research Project Number : 18H05535 Researcher Number : 50314175

【Purpose of the Research Project】

Today, Particle Physics and Cosmology are in a big turning point. The standard model of Particle Physics is well verified in a wide energy range up to TeV with the development of accelerators. Standard Cosmology describes Nucleosynthesis in the evolution of our universe, and firmly establish the existence of dark matter and dark energy. However, Standard Model and Standard Cosmology can not explain the origins of asymmetry between matter and anti-matter in our universe, the origin of inflation, the unified picture between forces and particles consisting of matter. To understand a picture from the beginning of our universe to the present, we must innovate a novel concept of Particle Physics and Cosmology. We challenge to build the new concept of Particle Physics and Cosmology by studying "neutrinos" that are the essential key particle to address these unresolved problems.

【Content of the Research Project】

We proceed with the world's best neutrino experiments: Super-Kamiokande, T2K, and IceCube, and we study neutrino oscillations, explore CP violation, and advance neutrino astronomy. Furthermore, in order to investigate the Grand Unification Theory and the initial state of our universe, we search for proton decay, measure neutrino mass from observation of Cosmic Microwave Background (CMB), and search for the signal of inflation (primitive gravity wave). In addition, we also study the Majorana nature of neutrinos.

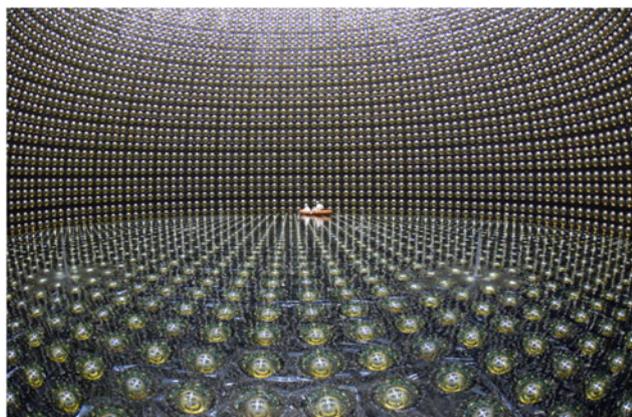


Fig-1 : Super-Kamiokande Detector

In order to realize the next-generation neutrino

experiments, we proceed with the development of basic technologies of Hyper-Kamiokande and IceCube Gen 2 experiments. With neutrinos, our research integrates particle physics, nuclear physics, cosmic rays, and cosmology.

【Expected Research Achievements and Scientific Significance】

【Development of neutrino physics】:

Determination of neutrino oscillations with high precision. Adding absolute neutrino mass and the number of generations, we advance understanding of the origin of neutrino mass and mixing.

【Evolution of neutrino astronomy】: We study Cosmic Neutrino Background, and observe neutrinos from sun, supernovae, galactic extraterrestrial objects, and AGN.

【Great Unified Theory (GUT)】: We search for the proton decay as an evidence of unification. By examining the symmetry between quarks and leptons, the GUT models are constrained.

【Elucidation of the evolution of our universe】: We have a big discovery potential to primitive gravitational waves, the origin of asymmetry between a particle and an anti-particle, dark matters, the B mode polarization of CMB.

【Key Words】

Neutrino: Neutrinos are elementary particles, similar to electrons but with no electric charge. There are three types of neutrinos. Non-zero neutrino mass was discovered by Super-Kamiokande. Neutrinos change their types through a phenomenon called "neutrino oscillation". Study of neutrino oscillations has advanced understanding nature of neutrinos.

【Term of Project】 FY2018-2022

【Budget Allocation】 1,129,900 Thousand Yen

【Homepage Address and Other Contact Information】

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**Title of Project : Materials Science on mille-feuille structure
- Development of next-generation structural
materials guided by a new strengthen principle -**

Eiji Abe

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

Research Project Number : 18H05475 Researcher Number : 70354222

【Purpose of the Research Project】

In order to solve the energy problem and realize a sustainable society, one of the prominent issues in materials science is to develop high-strength, light-weight structural materials. In our research project, we establish the “Kink strengthening phenomenon” as a universal strengthen principle, which has been firstly discovered in the LPSO-structured Mg alloy that revealed unusual high-strength beyond theoretical predictions. The LPSO structure can be generally viewed as “Mille-feuille structure”, in the sense that they are constructed by alternate stacking of microscopic hard- and soft-layer. Establishing a universal kink principle applicable to any mille-feuille structures will lead to a new academic, innovative area. Furthermore, based on the established “kink strengthening principle”, we will be able to design new alloys including Ti and Al alloys and further new polymer materials, providing an exciting opportunity for the development of next generation structural materials.

【Content of the Research Project】

Since kink formation and strengthening are not fully understood yet along with the existing solid deformation theory, it is indispensable to provide cross-disciplinary opportunities beyond the conventional frameworks, in order to establish a new academic field “Materials Science of a Mille-feuille structure”. In our research project, researchers participate across the wide research fields that are indispensable for the present tasks, the major three of which are “Materials synthesis (monozukuri)” “Solving the kink mechanism (elucidation of fundamental properties)” “Theory construction (universal principle/concept)”. We will be all together to form “Japan National Team” to tackle these challenging issues, creating a new universal academic field.

There are four research groups in our project. In **A01 group**, along the experiences with the LPSO-type Mg alloys, we will attempt to develop novel Mg alloys having various mill-feuille structures. In **A02 group**, we will try to elucidate the kink mechanism by performing mechanical experiments, advances structural measurements and computation modeling. In **A03 group**, a kink

strengthening theory will be constructed under the effective collaborations between multiple fields including materials science, mechanics, physics and mathematics. In **A04 group**, we will try to develop and synthesize novel metal- and polymer-base Mille-feuille materials according to a proposed kink strengthening theory.

【Expected Research Achievements and Scientific Significance】

- ① Establishing a novel strengthening principle of the Millefeil structure makes it possible to develop higher strength structural materials including new Mg, Ti and Al alloys, and further polymer based materials, contributing to an establishment of a energy-saving, sustainable society.
- ② Establishment of the systematic kink strengthening theory of the Millefeil structure is engraved in history as a new material strengthening method, and hence leads to worldwide reputation in a material science field.
- ③ Elucidation of the kink strengthening mechanism, based on the hierarchical structure science from the atomic level to the mesoscopic structures, brings out a drastic extension into a new solid mechanics that includes novel geometry and non-linear elastic theory.
- ④ Establishment of a new academic field “Materials Science of a Mille-feuille Structure” brings a great influence on wide basic-research fields, as well as an effective growth of the engineering fields and the relevant industry.

【Key Words】

Mille-feuille Structure: A microscopic layered structure constructed by an alternate stack of hard-layer (strongly-bonded) and soft-layer (weakly-bonded). It is named after “Mille-feuille cake”, which is composed of a pie layer (hard layer) and a cream layer (soft layer).

【Term of Project】 FY2018-2022

【Budget Allocation】 1,179,000 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Clustering as a window on the hierarchical structure of quantum systems

Takashi Nakamura
(Tokyo Institute of Technology, School of Science, Professor)

Research Project Number : 18H05400 Researcher Number : 50272456

【Purpose of the Research Project】

We aim to understand the formation mechanism of the hierarchical structure of quantum particles, from quarks to molecules (Fig.1). For this purpose, we integrate our research activities on hadron, nuclear, atomic physics, and molecular science, where Japan has played leading roles, and establish a research consortium to fill the large gaps among the conventional research fields. A variety of novel clustering phenomena will be primary targets of the research, which will clarify not only universal phenomena and physical laws, but also characteristic features of each hierarchy. We thus open a new research field to investigate the origin of hierarchies of matter.

【Content of the Research Project】

The quantum world has a hierarchical structure, from quarks to molecules (Fig.1). Each hierarchy is characterized by its unit particles and interactions between them. The unit particle, composed of lighter particles, is called a cluster. Recently, as shown in Fig.1, “Semi-hierarchy” lying between the conventional hierarchies, and its constituents, novel clusters, have drawn much attention. Such clusters may have universality across different hierarchies, and thus can provide a key to understand the hierarchical structure. As shown in Fig.2, Groups A,B,C will investigate clusters and interactions between them in each hierarchy. Group C, in addition, will explore quantum simulators to understand the clustering phenomena more generally. Group D will develop relevant theories. With this combined expertise, we expect to understand the underlying mechanism of the hierarchical structure.

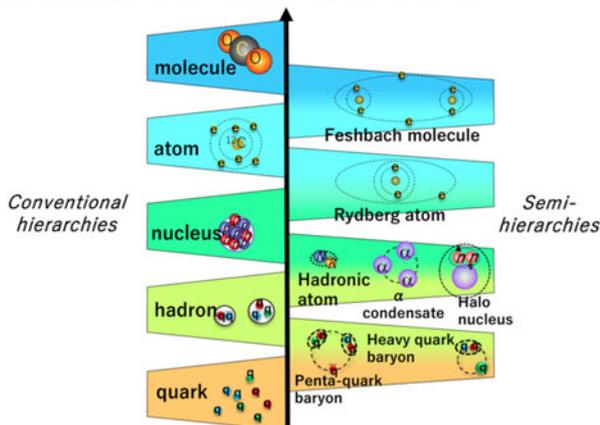


Fig.1 Hierarchical structure of matter

Connecting Hierarchies

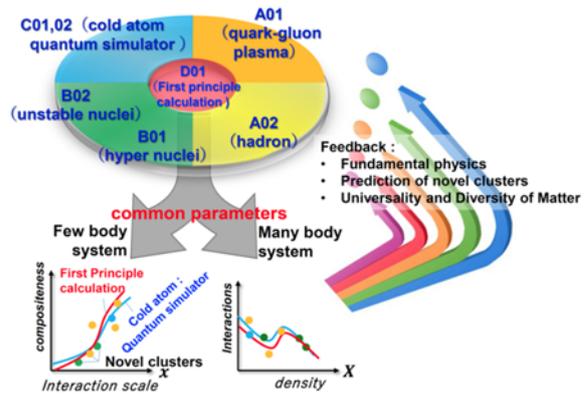


Fig.2 Scheme of this project

【Expected Research Achievements and Scientific Significance】

Novel clusters in semi-hierarchies will be observed and established. In addition, the interactions between the novel clusters will be investigated. Theories will play important roles in understanding the interactions from first principles. Quantum simulators using ultra-cold atom experiments will be one of the significant achievements. A semi-hierarchy with mixed configurations can be analyzed by quantum simulators, which will allow us to understand the phenomena in a more unified way. We thus expect to find physics phenomena and laws universally applicable to multiple hierarchies. In this way, we will open a new research field connecting the multiple hierarchies, from quarks to molecules, through the study of clustering phenomena.

【Key Words】

- Cluster:** A unit particle of the respective hierarchy, composed of lighter particles.
- Semi-hierarchy:** A hierarchy between two conventional hierarchies, often characterized by weakly (un)bound systems, strong pairing, mixed configurations, showing some universal features.
- Quantum simulator:** Simulators of quantum clusters to be realized by ultra-cold atom experiments.

【Term of Project】 FY2018-2022

【Budget Allocation】 1,169,700 Thousand Yen

【Homepage Address and Other Contact Information】

<http://be.nucl.ap.titech.ac.jp/cluster/>



Title of Project : High Entropy Alloys: Science of New Class of Materials Based on Elemental Multiplicity and Heterogeneity

Haruyuki Inui
(Kyoto University, Faculty of Engineering, Professor)

Research Project Number : 18H05450 Researcher Number : 30213135

【Purpose of the Research Project】

This project aims at establishing a new science concerning high-entropy alloys that exhibit new and peculiar materials properties by elucidating nonlinear interactions among various constituent elements through intensive and interdisciplinary cooperative research among research groups of various research fields within the project. ‘High-entropy alloys’ is defined in a narrow sense as equiatomic solid-solution alloys formed with constituent elements more than five kinds, the subjects of research have recently been expanded to include concentrated alloys with chemical compositions in the middle of multi-component phase diagrams, even they are deviated from the equiatomic compositions and contain precipitates of the secondary phase. Many of these high-entropy alloys of broader sense exhibit peculiar mechanical properties, such as abnormally high strength and high toughness at low temperatures, high strength retention at high temperatures, which are not observed in conventional alloys. These peculiar materials properties are considered to arise from the so-called ‘cocktail’ effects (nonlinear interactions among various constituent elements), and the identification of materials property expression behind the cocktail effects is one of the most challenging topics in materials science. Through establishing new scientific principle for controlling variety and inhomogeneity of elements, we aim at creating a new scientific area, in which the basis is established for developing new peculiar materials beyond conventional ones.

【Content of the Research Project】

In this research area, the following three research items are promoted cooperatively to establish a new scientific area with the concept of High-Entropy Alloys.

- Research Item A01: Identification of Materials Property Expression and Materials Development
- Research Item A02: Modelling and Designing of Materials Property
- Research Item A03: Controlling of Phase Stability and Microstructures

For all three items, several experimental and theoretical research groups will collaborate

closely together to promote the understanding of cocktail effects of high-entropy alloys.

【Expected Research Achievements and Scientific Significance】

Unlike conventional alloys (such as Ni- and Al-based alloys) that are developed with a particular principal element at a corner of the phase diagram, high-entropy alloys are to be developed in the middle of multi-component phase diagrams, which have been undiscovered. Many unknown alloys with excellent properties are therefore expected to be discovered. Some particular combinations of elements may generate a cocktail effect that is not predictable only from the combination, and we expect a paradigm shift to occur in materials development, so that a best combination of elements and their fractions is searched, departing from conventional ways with one particular principal element and some minor alloying elements.

【Key Words】

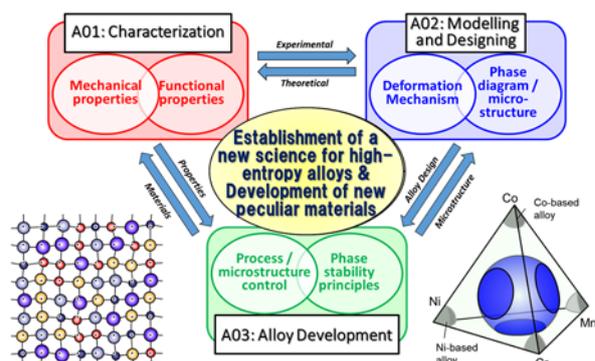
High-entropy alloy, Multi-component equiatomic alloy, high-order solid-solution, cocktail effect, materials strength, fracture toughness, solid-solution strengthening, phase stability, trap effect, variety of elements, inhomogeneity of elements

【Term of Project】 FY2018-2022

【Budget Allocation】 1,169,100 Thousand Yen

【Homepage Address and Other Contact Information】

<http://www.hightentropy.mtl.kyoto-u.ac.jp>





Title of Project : Toward new frontiers: Encounter and synergy of state-of-the-art astronomical detectors and exotic quantum beams

Tadayuki Takahashi
 (The University of Tokyo, Kavli Institute for the Physics and Mathematics of the Universe, Professor)

Research Project Number : 18H05457 Researcher Number : 50183851

【Purpose of the Research Project】

In recent years, a variety of fundamental scientific research fields have been established due to the production of various high-intensity quantum beams created by accelerators. However, these studies have been carried out independently and not enough effort has been made to share theoretical progresses and technological advances to other research fields. Based on the World-renowned advanced detector technology developed in Japan for space X-ray and gamma-ray observations, we will establish common theoretical frameworks and technological platforms and combine them with exotic quantum beams, namely negative muons, virtual photons and polarized RI beams. This will enable us to perform cooperative works in different research fields and develop novel methods. Furthermore, this will not only contribute to the area of fundamental sciences, but also towards new applications such as non-destructive 3D element analysis and medical applications.

【Content of the Research Project】

We aim to advance X-ray and γ ray imaging technologies and apply them to different research fields of quantum-beam experiments and to various other applications such as non-destructive analysis and medical imaging.
 (1) Precise spectroscopic measurements will be performed by detecting muonic X-rays combined with ultra-high resolution X-ray spectrometer and cadmium telluride (CdTe) semiconductor sensors. In addition, using the common framework of few-body theory combined with precise electro-magnetic spectroscopy of Λ hypernuclei utilizing real and virtual photons, hypernuclei in wide mass region will be studied to clarify the baryonic force and solve the puzzle of heavy neutron stars.
 (2) A nondestructive 3D imaging element analysis method will be established using muonic atom characteristic X-rays for bulk samples, and studies will be conducted on extraterrestrial

samples and archeology artifacts. Scientific research on muon catalyzed fusion will also be promoted based on a newly proposed reaction using high-intensity negative muon beam. Furthermore, by creating highly polarized RI beam without element dependence and replacing RI with atomic nucleus in a substance, material science research will be advanced by using the ultra-sensitive beta-radiation detected NMR method similar to μ SR.
 (3) Advanced detector system required for expanding the field as well as ultra-slow negative muon beam development will be carried out. Collaborative research with scientists in medicine and pharmacy will be initiated to develop in vivo 3D γ ray imaging device for small animals by applying CdTe semiconductor sensors to medical research on cancer stem cells.

【Expected Research Achievements and Scientific Significance】

Unprecedented precision experiments with newly developed detectors and exotic quantum beams will be realized in this program. A common theoretical framework of few-body systems will be established based on these experimental results. Especially, a research on exotic atoms using negative muons as "probes" has dramatically progressed, and application of muonic characteristic X-rays as ultra-sensitive non-destructive element analysis can finally be realized.

Highly-sensitive in vivo γ ray 3D imaging device with CdTe semi-conductor sensor technology will initiate studies of the properties and diversity of cancer cells in a tumor. Gathering researchers from various fields of expertise and generating ideas through brainstorming creates a "platform that facilitates the creation of new concepts".

【Key Words】

Negative muon: An elementary particle with similar properties as an electron but is 200 times heavier in mass.

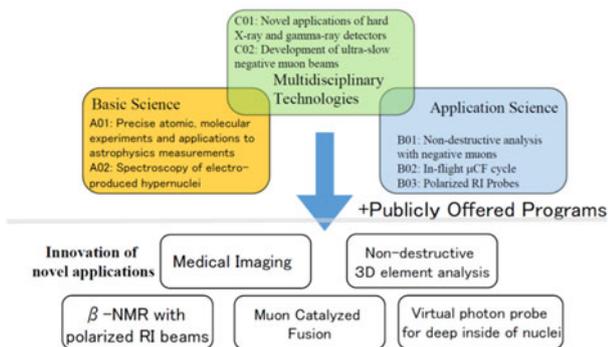
Cadmium telluride (CdTe): For 100-keV γ rays, it has 100 times higher detection efficiency than Si.

【Term of Project】 FY2018-2022

【Budget Allocation】 1,093,000 Thousand Yen

【Homepage Address and Other Contact Information】

[https://member.ipmu.jp/SpaceTech_to_Quantum Beam](https://member.ipmu.jp/SpaceTech_to_Quantum_Beam)



Organization of the Project

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