Title of Project：Frontiers of materials science spun from topology

Norio Kawakami
(Kyoto University, Graduate School of Science, Professor)

Research Project Number：15H05851　Researcher Number：10169683

【Purpose of the Research Project】

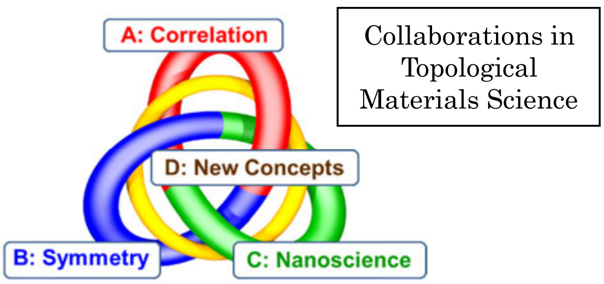
Focusing on topological nature of materials, we aim to develop novel quantum phenomena driven by interaction, symmetry of crystals and nanostructure of semiconductors, and explore exotic quasiparticles inherent in the topological quantum phenomena, thereby elucidating the underlying physics behind them.

Recent years have seen a tremendous growth of interest in topological quantum phenomena. However, quite a few issues still remain unexplored. In particular, (1) clarifying effects of **interactions** between electrons which would lead to diversity and functionality of materials, (2) exploring topological materials based on **symmetry** of crystals, and (3) systematic control of artificial topological phases in **nanostructured** systems, are indispensable for developing novel materials and establishing the fundamental concepts. This project systematically studies these issues at the frontiers of materials science.

【Content of the Research Project】

This project consists of four subprojects:

A: Topology and Correlation
B: Topology and Symmetry
C: Topology and Nanoscience
D: Topology and New Concepts



The subprojects A-C are closely related to real materials, and investigate strongly correlated systems, semiconductor systems and nanostructured systems. The subproject D consisting of a theory group aims to develop new concepts and stimulates collaborations among A-C.　We also have some theorists in A-C, who will do research in intimate collaboration with experimentalists.

Physical systems studied in this project are not restricted to ordinary topological insulators and superconductors, but widely include quantum systems, cold atomic systems, etc. where topological phases emerge.

In this project, we put particular emphasis on nurturing young researchers and promoting international collaborations: we introduce a special program to stimulate young researchers and international “alliance workshops”.

【Expected Research Achievements and Scientific Significance】

A significant feature of this project is our ambition to unify the basic concepts on topological phenomena found in different fields of condensed matter physics, and to provide a new versatile platform in materials science which can treat a variety of topological phenomena in the same framework.

Some concrete examples of the achievements we expect are:

1. Establishing topological phase transitions
2. Comprehensive understanding of topological insulators and superconductors
3. Realizing topological semimetals
4. Evidencing Majorana quasiparticles

By performing this project systematically, we will be able to solve the problems which have not been addressed in the preceding studies in each field, and stimulate the collaborations among different fields. This project will not only establish the basic notions of topological phenomena in condensed matter, but will also stimulate other research fields where the notion of topology will certainly become important in the near future.

【Key Words】

Topology, Materials science, Strong correlation, Symmetry, Nanoscience

【Term of Project】 FY2015-2019

【Budget Allocation】 1,003,600 Thousand Yen

【Homepage Address and Other Contact Information】

http://topo-mat-sci.jp/
tms-office@scphys.kyoto-u.ac.jp

Title of Project : Precise Formation of a Catalyst Having a Specified Field for Use in Extremely Difficult Substrate Conversion Reactions

Kazushi Mashima
(Osaka University, Graduate School of Engineering Science, Professor)

Research Project Number : 15H05795 Researcher Number : 70159143

【Purpose of the Research Project】

Synthetic organic chemistry is a fundamental science and technology that supports material sciences, such as drug development, polymer science, etc., by providing practical and efficient synthetic methods for the preparation of useful organic compounds. Organic chemists are expected to contribute not only to innovating and developing more practical and environmentally benign synthetic protocols but also to creating new compounds with higher functionalities or biological activities. For this purpose, development of new catalysts should play a key role, and the ultimate object of this program is to realize the precise formation of a catalyst with a specific scaffold to bring about innovation in this research field. Accordingly, this project is directed toward generating new catalysts with specific reactive fields that effectively enable extremely difficult substrate conversions. Examples of target reactions are direct functionalization of easily available hydrocarbons; direct conversion of CO_2, O_2, and N_2 into useful organic molecules; clean reactions without waste; and so on. As shown in Figure 1, a new research area – “Precisely Designed Catalysts with Customized Scaffolding”– will be developed by designing a catalytically active site surrounded by carefully designed scaffolds that enable control of reactivity and selectivity, activation of substrates, etc.

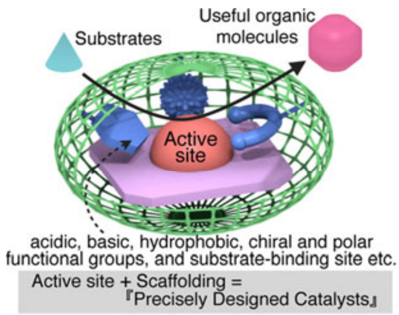


Fig 1. Strategy for Precisely Designed Catalysts.

【Content of the Research Project】

In this research area, as shown in Figure 2, the following four research items cooperatively collaborate with each other to introduce innovation in the field of catalytic synthetic organic chemistry. Intensive studies will be performed to install the appropriate functions of suitable steric and electronic properties into a specific field around a catalytically active site. Research Item A01: Development of Extremely Difficult Substrate Conversion; Research Item A02: Precise Formation of Transition Metal Catalysts with Molecular Scaffolding; Research Item A03: Precise Formation of Catalysts with Biomolecular Scaffolding; Research Item A04: Precise Formation of Catalysts with Large Scale Molecular Scaffolding.

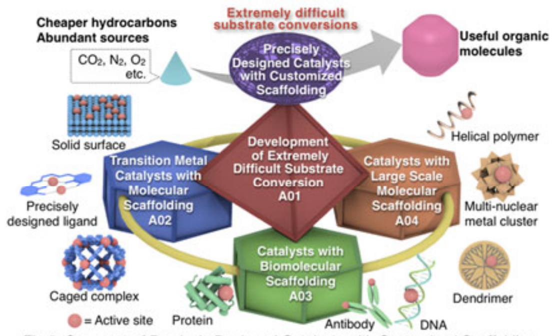


Fig 2. Concepts of Precisely Designed Catalysts with Customized Scaffolding and the Four Cooperatively-collaborating Research Items.

【Expected Research Achievements and Scientific Significance】

The creation of new catalysts with a specific field will open up new "synthetic organic chemistry", leading to the renovation of synthetic methodologies in industry and contributing to the realization of a sustainable society.

【Key Words】

Catalyst Having a Specified Field: A catalyst with a highly active site surrounded by various reactivity-controlling groups.

Extremely Difficult Substrate Conversion Reactions: Typical examples are direct functionalization of hydrocarbons; direct conversion of CO_2, O_2, and N_2 into useful organic molecules; and clean reactions without waste.

【Term of Project】 FY2015-2019

【Budget Allocation】 1,221,200 Thousand Yen

【Homepage Address and Other Contact Information】

http://precisely-designed-catalyst.jp/
mashima@chem.es.osaka-u.ac.jp

Title of Project : Science of Hybrid Quantum Systems

Yoshiro Hirayama
(Tohoku University, Graduate School of Science, Professor)

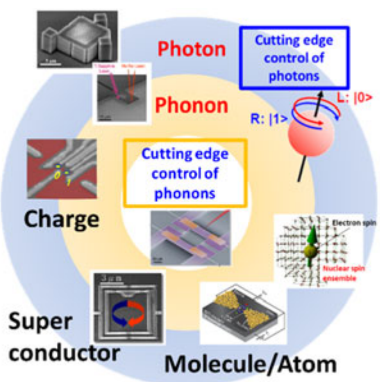
Research Project Number : 15H05866 Researcher Number : 20393754

【Purpose of the Research Project】

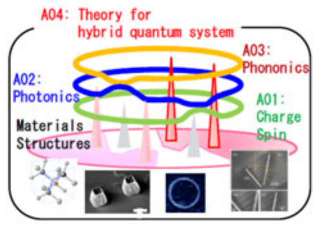
The purpose of this project is connecting the coherent manipulation of physics quantities for quantum enabled technology (QET) not for large scale quantum computation. A highly-sensitive metrology is received the most attention among the QET and the sensitivity can be enhanced by entanglement in the small-scale quantum hybridization. A quantum transducer coherently connecting various physics quantities is thus needed to create QET. We will establish the small-scale quantum coupling between different physics quantities by putting an emphasis not only on the *photon* but also the *phonon*, which has recently been remarkably developed.

【Content of the Research Project】

In the scheme of the project pursuing the fundamental physics of hybrid quantum systems, the A01 research will demonstrate the manipulation of the quantum coupling between a charge, spin, and nuclear spin. We will also study the coherent control of these physics quantities by photon and phonon. The A02 aims at the establishment of a cutting-edge photon-control and extends it to the quantum coupling between physics quantities and photons. We will clarify the interaction between materials and electro-magnetic waves. The A03 aims at the establishment of a cutting-edge phonon-control and extends it to the quantum coupling between physics quantities and phonons. We will attempt to create phonon-based transducer and hybrid phononic systems.



The A04 supports a better understanding of the experimental results and proposes a new direction for QET. Moreover, we clarify the limits of the quantum transducer and present some design rules. The theoretical studies will be used to create the project guidelines. We will collaborate with researchers in the field of nanomaterials and nanostructures because we will need new materials and structures for various quantum transducers.



【Expected Research Achievements and Scientific Significance】

This project focus on the small-scale quantum coupling between charge, cooper pair, spin, nuclear spin, photon, and phonon, that go beyond the existing frameworks, resulting in the highly-sensitive quantum metrology and QET. The new metrology will have a large impact on a wide range of fields. The establishment of a basic research area that is based on quantum coupling will pave the way for an attractive pure science like gravity detection. We will accelerate the world-wide movement towards the creation of QET in Japan.

【Key Words】

Nano-micro quantum system, New functional quantum material, Quantum effect, Quantum transducer, Quantum metrology, Quantum enabled technology, Solid-state physics, Quantum information, Charge, Spin, Nuclear spin, Photon, Phonon

【Term of Project】 FY2015-2019

【Budget Allocation】 1,045,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://quant-trans.org/hybridQS

Title of Project : J-Physics: Physics of conductive multipole systems

Hisatomo Harima
(Kobe University, Graduate School of Science, Professor)

Research Project Number : 15H05882 Researcher Number : 50211496

【Purpose of the Research Project】

Electrons are responsible for conduction phenomenon of material. An isolate electron has charge and spin of degrees of freedom. However, a variety of conduction phenomenon could not be understood, when we consider electrons just with charge and spin.

Orbital angular momentum of an electron in an atom couples its spin by the spin-orbit interaction, so a total angular momentum **J** becomes its characteristic. In solids, by the influence from the surroundings, the property of **J** changes into a multipole, which is microscopic freedom reflecting the atomic characteristic and the environment of the solid. The purpose of our project is to understand the various conduction phenomena by considering such a characteristic multipole.

With comprehensive cooperation, many researchers study together to establish the physics of conductive multipoles, and cultivate functional material leading to new applications. Besides, young researchers are trained to become key players in material science.

【Content of the Research Project】

Four groups both of planned researches and publicly invited researches promote the project.

A01: Correlation effect between localized multipoles and conduction electrons
-To study novel conduction phenomena produced by strong interactions between localized multipoles and itinerant conduction electrons.

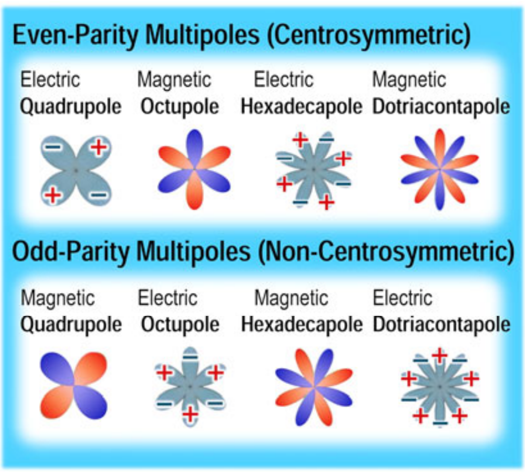


Figure: Multipoles. Odd-parity multipoles are allowed only in non-centrosymmetric case.

B01: Novel quantum phase with itinerant multipoles
-To study novel conduction phenomena, such as superconductivity, and ordered states relating with itinerant multipoles.

C01: Dynamical response from extended multipoles
-To search new dynamic response from multipoles, which are extended to several atoms, by using precise measurements.

D01: Development of strongly correlated multipole materials
-To develop new functional substances including high-temperature superconductors, where multipoles play a crucial role.

Odd parity multipoles allowed only in non-centrosymmetric case is expected to play a crucial role in a variety of systems. Therefore materials with a zigzag structure and a chiral structure are focused in research.

【Expected Research Achievements and Scientific Significance】

Unconventional conduction phenomena, such as ferromagnetic superconductors are clarified. Newly synthesized functional materials will be utilized as a huge responsive substance in multiferroics or spintronics fields. The concept of extended multipoles will be diverted to the field of functional molecules or biopolymers.

Focusing on multipoles together with young researchers, it brings a paradigm shift in solid state physics to contribute significantly to the science and technology innovation.

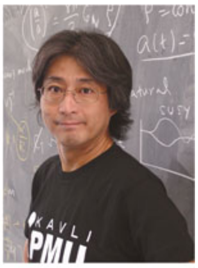
【Key Words】

spin-orbit interaction: interaction between the electron spin and orbital angular momentum in the central field, as a relativistic correction term derived from the Dirac eq.
total angular momentum: sum of spin angular momentum **S** and orbital angular momentum **L**, coupled by the spin-orbit interaction. It is usually expressed in **J**.
multipole: characteristic of the electrical or magnetic spatial distribution of electrons classified in point symmetry.

【Term of Project】 FY2015-2019

【Budget Allocation】 1,173,100 Thousand Yen

【Homepage Address and Other Contact Information】
http://www.jphysics.jp



Title of Project : Why does the Universe accelerate? -Exhaustive study and challenge for the future-

Hitoshi Murayama
(The University of Tokyo, Kavli Institute for the Physics and Mathematics of the Universe, Project Professor)

Research Project Number : 15H05887 Researcher Number : 20222341

【Purpose of the Research Project】

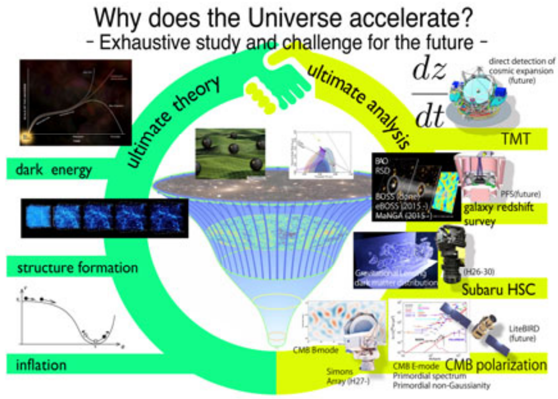
There are observational evidences for two periods of accelerated cosmic expansion, at the very beginning and the present. Since Newton and Einstein, gravity is known as an attractive force, hence can only “pull” the expansion to slow it down. What is “pushing” the Universe to speed it up? We often invoke “inflation” and Einstein’s “cosmological constant” as its *theory*, but they have many unnatural features and are far from satisfying explanations. The accelerated cosmic expansion is the mystery that goes to the basic foundation of physics.

The purpose of this research area is to understand the origin of the accelerated cosmic expansion, as well as its interplay with dark matter that competes with the acceleration to build galaxies and clusters of galaxies. To address this problem never encountered before, we propose to conduct research based on a comprehensive approach, ranging from the superstring theory to observation, experiments, and statistical analyses, and realize a quantum leap in this research area based on unprecedented data sets from the Subaru Telescope and others combined with novel data analyses and innovative theoretical ideas.

【Content of the Research Project】

To achieve the purpose, we organized theory units (A01-A03), observation units (B01-B04), and ultimate research units (C01, D01).

- A01 studies physical mechanism behind inflation based on gravity and particle theories as well as their testability.
- A02 studies mechanism for creating unknown particles including dark matter after inflation, characteristics and evolution of primordial fluctuations, and the structure formation as their consequences.
- A03 studies the origin of the current accelerated expansion, building the physical models of dark energy, possibilities of modified gravity, and their testability.
- B01–B04 take data at Simons Array CMB experiment (starting in 2017 with three telescopes), HSC imaging survey on Subaru (2014–19), and large-scale galaxy redshift surveys (BOSS/eBOSS), to constrain inflation and dark energy models with a ten-fold higher precision. In addition, we develop instruments, methodology, and software for future LiteBIRD CMB satellite, multi-object Prime Focus Spectrograph on Subaru, and direct measurement of cosmic acceleration on 30m TMT all led by Japan.
- C01 seeks ultimate theory of accelerated cosmic expansion from the superstring theory with top-down perspective.
- D01 develops ultimate tools of analyzing physical data to constrain physics behind accelerated cosmic expansion in a unified fashion exploiting multi-wavelength data.



【Expected Research Achievements and Scientific Significance】

During the proposed period, we will improve constraints on the energy scale of inflation with a search for primordial B-mode polarization in CMB, on time-variation of dark energy with a deep imaging survey, and on modified gravity and dark energy theories using the galaxy redshift surveys. We will maximize science by a synergistic development of theory and analyses of multi-wavelength data sets. We will thus create a new research area and aim for a full resolution of the mystery of accelerated cosmic expansion. It addresses age-old basic questions by humankind on the creation, fate, structure, and laws of the Universe.

【Key Words】

Accelerated cosmic expansion, quantum gravity, general relativity, inflation, dark matter, dark energy, neutrino, structure formation, cosmic microwave background, Subaru Telescope, Thirty Meter Telescope (TMT), LiteBIRD

【Term of Project】 FY 2015–2019

【Budget Allocation】 1,106,000 Thousand Yen

【Homepage Address and Other Contact Information】

http://acceleration.ipmu.jp

Title of Project : Interaction and Coevolution of the Core and Mantle : Toward Integrated Deep Earth Science

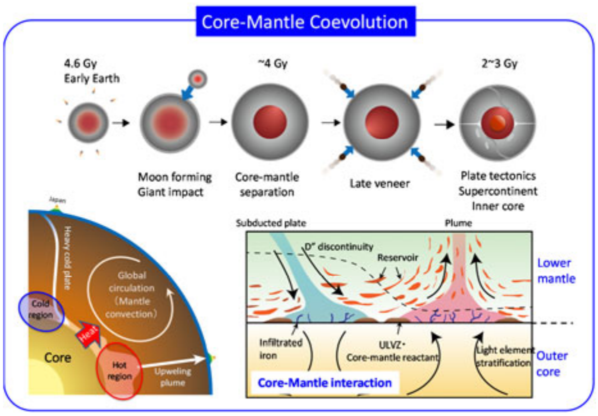
Taku Tsuchiya
(Ehime University, Geodynamics Research Center, Professor)

Research Project Number : 15H05826 Researcher Number : 70403863

【Purpose of the Research Project】

Recent observational and experimental investigations have significantly advanced understanding of the structure and constituent materials of the deep Earth. However, details of the chemical composition of the mantle, accounting for 80% of the volume of the entire Earth, and light elements expected to exist in the core, corresponding to the remaining 20%, have remained unclear for over 60 years. Seismological evidence has suggested a vigorous convection at the core-mantle boundary region, whereas geochemistry has suggested the presence of stable regions that hold the chemical signature of early Earth's formation 4.6 gigayears ago. In addition, the amounts and types of radioactive isotopes that act as the heat sources that drive the dynamic behaviors of the deep Earth are also still largely unknown. We will elucidate these unresolved mysteries of deep Earth science through comprehensive investigations of the interactions between the core and mantle by combining high-pressure and high-temperature experiments, microscale geochemical analysis, high-resolution geophysical observations, and large-scale numerical simulations.

【Content of the Research Project】



Our research target is to clarify the major unsolved mysteries in deep Earth science by focusing on the core-mantle interaction and coevolution by fusing different research fields that have developed individually in Earth and planetary sciences.

In our research program, we promote the study of several specific and important topics: (1) detailed compositional properties of the mantle and core including radioactive isotopes, (2) the relationship between the origin of the heterogeneities in the core-mantle boundary region and stable regions (primordial reservoir), and (3) chemical stratification of the outer core and the heterogeneity in the inner core. In order to perform these studies, an unprecedented and wide cross-disciplinary research structure consisting of five research units is organized (A01: Physical property measurement, A02: Geochemical analysis, A03: Geophysical observation, A04: Theory and computation, and B01: Integrated analysis), where researchers from a variety of different fields participate. Summarizing outcomes obtained from all the research units, we will create an integrated new and dynamic model/vision of deep Earth science.

【Expected Research Achievements and Scientific Significance】

The collaboration of world leading research fields in high-pressure Earth science, geochemistry, global seismology, and the more recently developed neutrino geophysics could make great contributions to inventing a new research direction in deep Earth science. This program could greatly enhance our understanding of the core-mantle coevolution system dominating Earth's internal dynamics and evolution. Development of talented human resources through the advanced researches is also of great significance in our program.

【Key Words】

Mantle: A region from a few 10 km to 2890 km depth in the Earth, consisting of solid rocks.
Core: A region from 2890 km to 6370 km depth (center of the Earth) in the Earth, consisting of metallic iron alloy. The biggest material boundary in the Earth is located between the core and mantle (named the core-mantle boundary).

【Term of Project】 FY2015-2019

【Budget Allocation】 1,091,100 Thousand Yen

【Homepage Address and Other Contact Information】

http://core-mantle.jp/
tsuchiya.taku.mg@ehime-u.ac.jp

Title of Project : Middle Molecular Strategy: Creation of Higher Bio-functional Molecules by Integrated Synthesis

Koichi Fukase
(Osaka University, Graduate School of Science, Professor)

Research Project Number : 15H05835 Researcher Number : 80192722

【Purpose of the Research Project】

Middle-size biomolecules (MW ca. 400-4000) such as natural products, glycans, peptides, nucleic acid drug, and etc have high chemical diversity and various biological activities. They are also termed as middle molecules, mid-size molecules, medium size molecules, and so on. Middle molecules have great potential as higher bio-functional molecules because of the following characteristics. Since middle molecules have relatively large surface area in comparison to small molecules, the strict and diverse molecular recognition is possible based on the multipoint interaction between middle molecules and target proteins, enabling both "lock and key" recognition in the binding pocket and the protein surface recognition. Some of middle molecules interact with several proteins simultaneously to dynamically control the signaling. In addition, some of middle molecules are membrane permeable and orally active.

However, the inherent structural complexity of middle molecules was an obstacle for the practical use of middle molecules, since the synthesis of them is often difficult and generally requires many reaction steps. Therefore, the present research project will achieve a highly efficient synthesis of bioactive middle molecules by an innovative synthetic strategy based on reaction integration. Further, novel bio-functional middle molecules will be developed by new strategies such as function integration.

【Content of the Research Project】

In this research project, bio-functional middle molecules will be developed based on the two strategies, i) efficient synthesis of bioactive natural products, ii) synthesis of hybrid middle molecules by function integration. The efficient synthesis of middle molecules by reaction integration will be also investigated.

In A01, efficient synthesis of bio-functional middle molecules such as glycans, nucleic acids, peptides, and lipids will be studied. Development of novel bio-functional middle molecules will be also investigated by function integration, i.e., conjugation of bioactive compounds, creation of novel bio-functional molecules possessing the π electron system compounds.

A02 aims the highly efficient synthesis of bioactive middle molecules such as complex natural products. A02 will also study the reaction integration based on novel concepts and techniques such as synthesis using living cells and chemo-enzymatic synthesis.

A03 will develop continuous reaction processes using micro-flow and one-pot syntheses as well as practical reactions for multi-step synthesis. Synthetic transformations allowed by micro-flow methods, such as very fast reactions using unstable reactive species, will be also investigated.

【Expected Research Achievements and Scientific Significance】

This research project will realize highly efficient processes by reaction integration to achieve the efficient synthesis of complex middle molecules. Since middle molecules have high potential as bio-functional molecules such as pharmaceutical agents and agrochemicals, this research project will lead innovative pharmaceutical drugs, diagnostic agents, and pesticides, e.g., effective immunoadjutants, synthetic vaccines, selective anti-cancer agents, environment-friendly pesticides, and etc.

【Key Words】

Middle molecule, natural product, glycan, peptide, π electron system compound, higher bio-functional molecule, reaction integration, micro-flow synthesis, continuous reaction process, multistep synthesis, catalyst, function integration

【Term of Project】 FY2015-2019

【Budget Allocation】 1,108,100 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.middle-molecule.jp
middle-molecule@chem.sci.osaka-u.ac.jp

Title of Project : Solar-Terrestrial Environment Prediction as Science and Social Infrastructure

Kanya Kusano
(Nagoya University, Solar-Terrestrial Environment Laboratory, Professor)

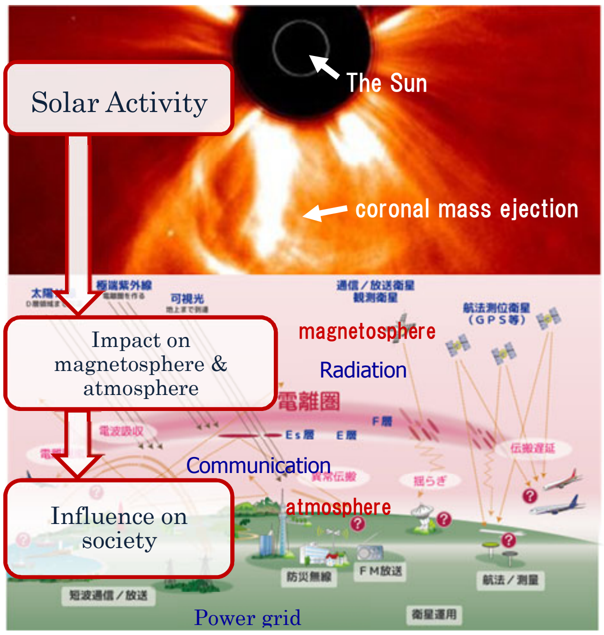
Research Project Number : 15H05812 Researcher Number : 70183796

【Purpose of the Research Project】

Over the last 50 years, space exploration and space utilization has seen a rapid spread. As a result, the dynamics of the sun and space has been found to have a significant impact on the global environment as well as human society. However, the mechanisms of solar explosion and the subsequent processes have not yet been fully elucidated. Therefore, the advanced information society will have potential risk to severe space weather disturbance caused by giant solar explosion.

On the other hand, the sunspot activity that causes the solar-terrestrial environment variability will be activated with a period of about 11 year cycle. However, the current solar cycle (Cycle 24) manifests as the lowest solar cycle in the past 100 years. Although many data suggested that the solar cycle variation may affect the weather and climate of the Earth, the causality between the solar activity and the variation of global environment is not yet clearly explained. Therefore, the role of solar activity in climate change is still greatly ambiguous.

This project aims to develop the synergistic interaction between the prediction research and the scientific research of the solar-terrestrial environment variation to establish the base of next-generation space weather forecast.



Various impacts of solar explosion on the social systems.

【Content of the Research Project】

This project coordinates the interdisciplinary research on the following subjects.
(1) Next Generation Space Weather Forecast: To develop a new space weather forecast system that may be utilized as a social infrastructure.
(2) Prediction of solar storms: To establish the prediction system of solar explosion based on the state-of-the-art observations and the physics-based models.
(3) Prediction of magnetosphere and ionosphere dynamics: To understand and predict the disturbance of space radiation, ionospheric storm, and geo-magnetically induced current.
(4) Prediction and understanding of solar cycle activity and the impact on climate: To elucidate the cause of solar cycle and the climate impact.
(5) Mathematical sciences for solar-terrestrial environment variability.

【Expected Research Achievements and Scientific Significance】

This study solves many scientific important issues of the solar-terrestrial environment, and achieves the following developments.
① The quantitative assessment of the severe space weather disasters.
② The contribution to the future space exploration and the guidelines of the heliospheric science mission
③ The development of prediction algorithm, which contributes also to the climate change projection.

【Key Words】

The sun, solar flare, coronal mass ejection, CME, solar cycle, magnetosphere, ionosphere, space weather, space climate, climate change, space radiation, geo-magnetic storm

【Term of Project】 FY2015-2019

【Budget Allocation】 649,400 Thousand Yen

【Homepage Address and Other Contact Information】

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