Title of Project: New Polymeric Materials Based on Element-Blocks

Yoshiki Chujo
(Kyoto University, Graduate School of Engineering, Professor)

Purpose of the Research Project
The main purpose of this research project is to establish new and innovative polymeric materials based on “element-blocks”. Recently, organic-inorganic hybrids that have effectively combined properties of organic and inorganic materials and organic polymer materials hybridized with various inorganic elements at the molecular level have been extensively studied as new functional materials, such as electronic device materials. In this research project, such concept of hybridization is applied to element blocks. New element blocks with a variety of elements are synthesized by several approaches including organic, inorganic, and organometallic reactions, which are polymerized, and the polymer integration is studied with respect to the regulation of interface and higher ordered structures in the solid states. Based on this strategy, we develop new innovative element-block polymer materials and establish the new theory of polymeric materials based on element-blocks (Figure 1).

Content of the Research Project
This research group is composed of four sub-groups which promote the research by close collaboration between them (Figure 2). A01 (Exploration of New Element-Blocks) deals with design and synthesis of new element-blocks, while in A02 (Polymer Synthesis Based on Element-Blocks) and A03 (Regulation of Interface and Higher Ordered Structures), polymerization of the element-blocks, and their nano-sized interface structures, higher ordered structures, non-bonding interaction of the polymers are studied, respectively. In A04 (Development of New Ideas and Collaboration), theoretical analysis of the element-block polymers is studied to gain new ideas. Collaboration based on new seeds and challenging ideas of element blocks is encouraged in this group.

Expected Research Achievements and Scientific Significance
In this project, not only the development of individual functional materials based on the idea of element-blocks, but also the establishment of a new theory concerning element-blocks, which can provide new ideas of molecular design and methodology of material synthesis are expected.

Key Word
Element-blocks: Building units of polymers with a variety of elements

Term of Project
FY2012-2016

Budget Allocation
1,161,100 Thousand Yen

Homepage Address and Other Contact Information
http://element-block.org
Title of Project: New Developments in Astrophysics Through Multi-Messenger Observations of Gravitational Wave Sources

Takashi Nakamura
(Kyoto University, Graduate School of Science, Professor)

Purpose of the Research Project

One hundred years ago, Albert Einstein's theory of general relativity predicted the existence of gravitational waves (GW). However, their effects are expected to be extremely subtle, and as a result they have not yet been detected. Now, a new generation of GW detectors are coming online in the US, Europe, and Japan. They should be ready to detect strong sources of gravitational waves – like the collapse of a heavy star into a supernova and black hole, or the coalescence of a neutron star binary – as early as 2016. Such powerful GW sources should also emit a wide variety of other "messengers": X-rays, gamma-rays, visible and infrared light, radio waves, and neutrinos. The goal of this new innovative area is to enable both coincident and follow-up observations of these messengers through collaborative efforts in Japan, and by doing so to thereby extend man's understanding of the universe via: (1) confirmation of Einstein's 100-year-old prediction, and (2) observationally establishing the origin of the substances which comprise both humans and the world around them.

Content of the Research Project

To conclusively demonstrate the observation of gravitational waves, we need not only detection of the gravitational waves themselves but also counterpart observations. Our innovative research area consists of three categories of observations as well as two types of gravitational wave study: X-ray/gamma-ray (A01), optical/radio (A02), neutrino (A03), gravitational wave data analysis (A04), and theoretical GW research (A05). We wish to probe the inside of gravitational wave sources with the cooperation of these research projects.

Expected Research Achievements and Scientific Significance

Once gravitational waves are observed, signals from other messengers are expected. In the case of the coalescence of a neutron star binary, gravitational wave data analysis will roughly suggest the arrival direction. A rapid follow-up of X-ray and/or gamma-ray observations will narrow down the arrival direction, while optical follow-ups should allow identification of the host galaxy. In case of a supernova in our own galaxy, coincident detection of neutrinos would give certain confirmation of a gravitational wave signal. These simultaneous measurements – the only known techniques to look into the very heart of a collapsing star – will provide vital knowledge of these astronomical objects.

Key Words

General Relativity: General theory of gravity (which includes Newton's gravity), proposed by A. Einstein at 1915. Based on this theory, there are many ideas regarding what happens in strong gravity fields, but experimental data is lacking. Gaining observational GW data will likely provide the key to creating a modern, 21st century unified theory which includes gravity. Gravitational Wave: Wave in the gravity field which was predicted by Einstein according to general relativity. Gravitational waves should propagate at the speed of light and distort space-time, but the direct measurement of this propagation has not yet been established.

Term of Project

FY2012-FY2016

Budget Allocation

910,500 Thousand Yen

Homepage Address and Other Contact Information

http://www.gw.hep.osaka-cu.ac.jp/gwastro
Title of Project: Development of Molecular Robots equipped with sensors and intelligence

Masami Hagiya
(The University of Tokyo, Graduate School of Information Science and Technology, Professor)

[Purpose of the Research Project]
This project aims to establish the field of molecular robotics by means of promoting the engineering of molecular devices up to the level of molecular systems. Molecular robotics requires the systematic integration of scientific and technological accomplishments of various fields, especially those of chemistry and DNA nanotechnology. The methodologies of systems science, such as control theory and numerical simulation, play an important role in the design and implementation of molecular robots.

To achieve this aim, we focus on a revolutionary way of artifact production, a bottom-up methodology in which material molecules are programmed so that they become a desired product by a self-assembling process.

Artifacts will be more useful if they provide not only atomic-level resolution of shape but also advanced functions such as self-repair and self-reconfiguration at the molecular level. Such artifacts will be expected to make a large impact on solving problems in healthcare, food and energy.

[Contents of the Research Project]
A robot is an artifact that can exhibit intelligent behaviors by means of multiple sensing-processing-actuating cycles. It requires the facilities of sensors, actuators, and intelligence as well as a body to integrate these facilities. In molecular robots, those elements must be realized in the form of functional molecules (Fig.1). To achieve this, it is necessary not only to develop each element, but also to develop technology to integrate and organize the elements into one consistent system. All the component elements of the molecular robot must be assembled by bottom-up self-assembly, and behaviors of the robot must be controlled based on chemical reactions.

To realize this concept, the project is divided into four subprojects: (A01) subproject aiming at developing molecular sensing devices; (B01) subproject aiming at developing methodology to implement molecular control circuits; (C01) subproject to develop a micron-sized amoeba-like prototype; and (D01) subproject to develop a millimeter-sized slime-like prototype.

Some additional projects will also be recruited for the purpose of reinforcing necessary elements to realize the prototypes and also to search for their possible applications.

[Expected Research Achievements and Scientific Significance]
The evolutionary process of the molecular robot will be something similar to that of the evolution of living organisms. Many technological hurdles await us, but when these hurdles are overcome, new possibilities will arise. Ultimately, the process moves toward hybridization of molecular and electric technologies (Fig.2).

[Key Words]
Molecular Robotics: Methodology to integrate and program molecular devices as a system

[Term of Project] FY2012-2016

[Budget Allocation] 1,038,800 Thousand Yen

[Homepage Address and Other Contact Information]
http://molbot.org/shin-gaku/
Title of Project: Nuclear Matter in Neutron Stars Investigated by Experiments and Astronomical Observations

Hirokazu Tamura
(Tohoku University, Graduate School of Science, Professor)

Purpose of the Research Project

Neutron stars are extremely dense stellar objects whose core part is made only of baryons (neutrons and other particles) without electrons. Our project aims at revealing this unknown matter by combining experiments on the earth and astronomical observations from the space through theoretical studies.

As illustrated in Fig. 1, we experimentally study strangeness nuclear physics at J-PARC, neutron-rich nuclei at RIBF in RIKEN, ultra-cold atomic gas, and also observe neutron stars using X-ray satellites such as ASTRO-H. Then we combine those results through theoretical studies to uniquely determine the equation of state (EOS) of nuclear matter. Then various types of matter in the neutron stars and the structure of the neutron stars will be revealed.

Expected Research Achievements and Scientific Significance

As mentioned above, we will be able to uniquely establish the EOS of nuclear matter, which has been one of the dreams in nuclear physics. Then the structure of the neutron stars and various types of matter inside them will be understood, and the long-standing questions such as existence of strange hadronic matter and superfluid neutron matter will be answered. The mechanism of production and cooling of neutron stars will be also elucidated.

Furthermore, this project will lead to a creation of a new type of science for matter beyond atomic/molecular physics, condensed matter physics, chemistry, and plasma physics.

Content of the Research Project

(A) In order to investigate the high density region in the central part of the neutron stars, where strange quarks are expected to appear, we study strangeness nuclear systems (hyper-nuclei) and determine the hyperon-nucleon interactions to be used as an input for the EOS.

(B) In order to understand low/medium density neutron matter in the outer region of the neutron stars, we investigate properties of neutron-rich nuclear matter and thin neutron matter through various studies of neutron-rich unstable nuclei. We also investigate laser-cooled ultra-cold Fermi gas systems, of which properties are similar to thin neutron matter in the crust of the neutron stars.

(C) Both of the mass and the radius of the neutron star would strongly restrict and/or confirm the EOS. However, direct measurement of the radius has not been achieved yet. Using X-ray observatory satellites such as ASTRO-H with new X-ray detectors, we will obtain direct data on the radius for several samples.

(D) The theory group studies related subjects on nuclear/hadron physics, cold atomic systems, and astronomical physics to analyze/interpret results of (A), (B), (C). The best EOS will be constructed from (A) and (B), and then confirmed by the radius data (C). Exotic neutron-star matter such as various baryonic superfluid and pasta-like matter will be also investigated.

Key Words

Neutron star: Extremely dense stellar object which remains after supernova explosion.
Nuclear Matter: Matter in a nucleus consisting of baryons (such as neutrons) without electrons.

Term of Project

FY2012-2016

Budget Allocation

1,079,300 Thousand Yen

Homepage Address and Other Contact Information

http://lambda.phys.tohoku.ac.jp/nstar/tamura@lambda.phys.tohoku.ac.jp
Title of Project: A multifaceted approach toward understanding the limitations of computation

Osamu Watanabe
(Tokyo Institute of Technology, Graduate School of Information Science and Engineering, Professor)

Purpose of the Research Project
The goal of this project is to establish strong mathematical foundations for understanding the limits of computation. In particular, we will develop various fundamental results that would suggest the next step toward resolving the P≠NP conjecture.

Mathematics has traditionally been regarded as the “language” of the sciences. In recent times Computation has become another “language” common to various scientific fields. Although computation is pervasively in our daily lives, our understanding of computation is still partial. One typical example is the limit of the efficiency of algorithms. For solving a given computational problem, there are various algorithms, and designing efficient algorithms is one of the important subjects in computer science. On the other hand, one can easily expect that there should be a limit; for any problem, there should be a theoretical limit of improving its algorithmic efficiency. Unfortunately, however, we have not been able to understand such limits for most of the problems around us. An important question on the limits of computation is the P≠NP conjecture. Our goal is to develop techniques and theories for pushing the frontier of our understanding of the inherent limitations of algorithms, thereby advancing our understanding of computation.

Content of the Research Project
The 1990’s saw various new techniques and exciting results on the limits of computation. Throughout the 2000’s, these techniques were continually sharpened. Based on these efforts, we may soon enter the stage of expecting some big breakthrough results toward understanding the limits of computation. In this project, we will investigate these techniques and relationships among them and derive some multiple theories suggesting the next steps toward a big breakthrough. Motivated by this goal, world leading experts on various aspects of computations are uniting to form a research cloud consisting of nine groups investigating computational limits from different view point. By intensively collaborating each other, we will explore the potential of various technique for bounding the limits of computation. Specifically, for typical techniques for analyzing computational lower bounds, we shall (i) give new interpretation as to how and why through the discussion by researchers with different scientific viewpoints, (ii) derive new relationships between these techniques and obtain new applications, and (iii) apply this knowledge to get innovative results, pushing the frontier of our understanding of the limits of computation. This is our research framework of this project.

Expected Research Achievements and Scientific Significance
We believe that the above explained research framework is strong enough to obtain many fundamental results, from which we may see new steps toward the P ≠ NP conjecture. Such results must reveal some aspects of computation: thus, although these are purely mathematical, they may lead some novel algorithms, new computational concepts, and even new areas for computation.

Key Words
NP problem: A computational problem such that for each given input, checking its solution candidate is relatively easy. This type of problem can be found in almost all fields of the sciences.
P ≠ NP conjecture: A conjecture claiming that there is some NP problem such that no efficient algorithm can compute its solutions.

Term of Project
FY2012-2016

Budget Allocation
536,500 Thousand Yen

Homepage Address and Other Contact Information
http://www.ai.ics.saitama-u.ac.jp/elc/en/elc-office@is.titech.ac.jp
Title of Project : Chemical conversion of solar energy by artificial photosynthesis: a breakthrough by fusion of related fields toward realization of practical processes

Haruo Inoue
(Tokyo Metropolitan University, Department of Applied Chemistry, Professor)

[Purpose of the Research Project]
“Energy crisis” in global scale in near future is now becoming to be accepted to be inevitable. It is anticipated that fossil oil shall be consumed up within ca. 60 years. It should be most required to realize a renewable energy system, artificial photosynthetic one. It enables to convert solar energy into chemical energy (fuel) which can be utilized in a desired amount at a desired time. The artificial photosynthesis has been a “dream of human being,” but now is becoming the most crucial issue to be realized for the sustainable society. For getting to its realization, however, much breakthrough in the corresponding science and technology should be further required, though many Japanese scientists in the artificial photosynthesis-related fields have been leading their edges. On the basis of those pioneering achievements, this project challenges to realize artificial photosynthesis through a multiple-cross-fertilization among all the corresponding fields with all members of the project.

[Content of the Research Project]
To realize artificial photosynthesis, establishing redox reaction systems with water as electron donor should be indispensable. Research strategy of 1) learning and understanding natural photosynthesis, 2) mimicking nature, and exceeding nature will be adopted to organize the project team with the following four sub-groups.

1) Development of artificial photosynthetic system with efficient light harvesting devices (A01 group): (Learning and understanding natural light harvesting system to lead to artificial one which can be effectively coupled with catalytic center)

2) Development of artificial photosynthetic system with efficient photocatalytic oxidation of water (A02 group): (Learning, understanding, and being inspired by the structure and mechanism of PSII in natural photosynthesis to establish artificial system of photocatalytic oxidation of water)

3) Development of artificial photosynthetic system with efficient hydrogen evolution (A03 group): (Efficient hydrogen formation by electrons from water)

4) Development of artificial photosynthetic system with efficient photochemical reduction of carbon dioxide (A04 group): (Efficient photochemical reduction of carbon dioxide into CO, formic acid, and alcohol)

[Expected Research Achievements and Scientific Significance]
In this project, a forum on artificial photosynthesis among the leading scientists will be organized to realize chemical conversions of solar energy with water as electron donor and to develop them into practical processes through multiple-cross-fertilization among all the related area with all-Japan members of the project team. International open-innovation on artificial photosynthesis will be created. Each leading scientist is situated on the crossing point of the vertical axis of each sub-group with distinct object and the horizontal one of fundamental discipline with characteristic methodology. It induces the multiple-cross-fertilization among the discipline and the methodology to focus on the targeting object, which will promisingly lead to establish artificial photosynthesis with water as electron donor.

[Key Words]
Artificial photosynthesis: Solar energy and water store the energy in chemical substances such as hydrogen and alcohol. Renewable energy: Energy which can be continuously supplied by nature.

[Term of Project] FY2012-2016
[Budget Allocation] 750,700 Thousand Yen
[Homepage Address and Other Contact Information]
http://artificial-photosynthesis.net/
Title of Project: Plasma Medical Innovation

Masaru Hori  
(Nagoya University, Graduate School of Engineer, Professor)

Purpose of the Research Project

Plasma consists of a variety of reactive species (ions, electrons, radicals and emitting photons). In discharge plasmas, these reactive species are generated via ionization and dissociation of gaseous molecules through collisions with accelerated electrons. Due to enhanced reactivity of these reactive species, plasma has been employed as major tools for material processes including formations of ultrafine structures and functional layers, which are indispensable as key manufacturing technology for advanced industries and eventually have taken a role as core technology to support the state-of-the-art advancement of scientific frontiers.

Meanwhile, in the last decade, technological progress has been made to generate non-thermal low-temperature plasma in atmospheric-pressure gas and in liquid, in which the gas temperature is maintained at a room temperature. Recently the non-thermal plasmas have been applied to medical treatments, in which remarkable effects have been found in apoptotic behaviors of cancer cells, skin-disease therapy and wound healing, and thus the plasma is expected to bring significant innovations in medical science and technologies.

The goal of our research project is to create “Plasma Medical Innovation” as a novel academic field for development of innovative technologies in medical treatments through establishment of scientific basis involved in plasma interactions with biomolecules, cells and living bodies. In particular, our research project is to place special emphasis on studies and systematization of the interactions based on “plasma science” and “molecular biology”.

Content of the Research Project

For creation of the field “Plasma Medical Innovation” and leading the worldwide research activities, it is of key significance to establish following schemes to evolve the novel academic field via utilizing unique scientific achievements gained in the “advanced plasma-process science”, which has lead the industries worldwide, for development of medical science and molecular biology.

1. Development of unique plasma sources and diagnostic technologies through establishment of methodologies to study the interactions between plasma science.
2. To study the interactions on the atomic and the molecular scales based on molecular biology for theoretical systematization.
3. Evolution of the novel academic field via systematic research activities that cover interaction studies and experiments on animals, evaluation of side effects (toxicity), and establishment of international guidelines to assure safety as medical treatments.

Systematization as the plasma medical science shall be attained via collaborative studies in 1) and 2). Furthermore, innovative medical technologies with novel plasma sources and diagnostic systems shall be developed through systematic research activities via 3) together with 1) and 2).

Expected Research Achievements and Scientific Significance

The achievement of our goal is expected to contribute significantly to a) enhancement and promotion of academic level of our nation and moreover b) substantial promotion of “the life innovation” through medical innovations and evolutions that are attained via development of the novel medical technologies alternative to the conventional ones.

Key Words: plasma medicine, molecular biology, plasma interactions with living body, life innovation

Term of Project: FY2012-2016
Budget Allocation: 1,131,800 Thousand Yen

Homepage Address and Other Contact Information:
http://plasmamed.jp
secretariat@plasmamed.jp
Title of Project: Stimuli-responsive Chemical Species for the Creation of Functional Molecules

Yohsuke Yamamoto
(Hiroshima University, Graduate School of Science, Professor)

[Purpose of the Research Project]
Recent developments in the field of “elemental science” based on the efficient utilization of the intrinsic character of each element are remarkable. A variety of fascinating compounds having unusual bonding schemes and structures have been spectroscopically characterized or even isolated owing to the creative design of ligands and substituents. Representative examples include those containing silicon-silicon triple bonds, π-single bonds, five- and six-coordinate carbons, and nucleophilic borons. A notable point is that most of them are highly stimuli-responsive molecules and are thus readily converted to high-energy species that possess high potential for molecular functions.

In this project, we aim to establish the fundamentals and explore applications of such “stimuli-responsive chemical species” through joint studies between leading chemists in various research fields including organic, inorganic, materials, theoretical, and biological chemistry, with the goal of creating new types of functional molecules.

[Content of the Research Project]
The valence shell of main group elements of the third and lower rows of the periodic table is distant from the nuclei and high in energy. In addition, the size of the s-orbital and the p-orbitals is very different. Thus, the hybridization of these orbitals is generally difficult. This partially contributes to the transition metal-like properties of such elements. Innovative functional molecules are to be created by joint research involving main-group element and transition metal chemistry. Indeed, main group elements of the third row and transition metals are known to play important cooperative roles at the active sites of enzymes in essential biological processes.

Molecular compounds with new functionality derived from characteristics inherent to each element are targets in this Scientific Research on Innovative Areas project. New reactions, molecules with new functions, and new catalysts are to be developed through joint research studies, and the elucidation of enzyme reaction mechanisms and the development of artificial enzymes are to be achieved. To advance the scientific research project, we have set up the following four sub-projects.

A01: Stimuli-Responsive Chemical Species for the Development of Functional Reagents. Highly polarized chemical bonds using main-group elements are to be designed and prepared. The stimuli-responsive chemical bonds are expected to activate inert small molecules such as CO₂.

A02: Stimuli-Responsive Chemical Species for the Development of Functional Materials. Compounds with unusual π-bonds such as silicon-silicon triple bonds and π-single bonds are to be designed and synthesized using kinetic stabilization methods.

A03: Stimuli-Responsive Chemical Species for the Development of Functional Catalysts. New types of molecular catalysts are to be developed and new ligands designed utilizing electronically flexible main-group elements.

A04: Stimuli-Responsive Chemical Species for the Elucidation of Enzymatic Processes. The discovery of new stimuli-responsive chemical species and their application for the elucidation of enzyme reactions are to be explored using methods of advanced structural biochemistry and quantum chemical calculations.

[Expected Research Achievements and Scientific Significance]
The invention of new functional molecules is one of the utmost important tasks of chemistry. With the clear-cut concept of “stimuli-responsive chemical species”, it is highly anticipated that the newly discovered reactions, properties, and functions will provide the basis for breakthroughs in socially important issues including renewable energy and environmental problems.

[Key Words]
Stimuli-responsive Chemical Species, High-energy Species, Functional Molecules.

[Term of Project] FY2012-2016

[Budget Allocation] 1,118,200 Thousand Yen

[Homepage Address and Other Contact Information] http://www.strecs.jp
Title of Project : Interdisciplinary Study on Environmental Transfer of Radionuclides from the Fukushima Daiichi NPP Accident

Yuichi Onda
( University of Tsukuba, Faculty of Life and Environmental Sciences, Professor )

[Purpose of the Research Project]
Massive earthquake attacked the eastern Japan on March 11 2011. It triggered violent tsunami that damaged the Fukushima Nuclear Power Plant. A large amount of gamma-emitting radionuclides were released into its surrounding area and also circulated globally with atmospheric diffusion process. After more than a year since the accident, an interdisciplinary study on fallout radionuclides for long–term estimation will become more important than the investigation for basic countermeasures such as short-term estimation and decontamination.

With the variety of circulation and interaction processes, transfer of fallout radionuclides will become a serious issue in the future. The forms of transfer include entrainment from the ground surface, sediment transfer with associated radionuclides to rivers and reservoirs, and radionuclide migration to forests, crops, marine and terrestrial ecosystems.

Radioactive contamination is a complex and unprecedented problem that will not be resolved by a single tackle in each field. Based on the many fields of geoenvironmental sciences, establishment of a new and cross-sectional study area with radiochemical and nuclear gauging technology is required.

Researchers join this project with their wisdom in the long-term radionuclide migration in the environment and the estimation of environmental dynamics. Through these studies we will try to establish the formation of the world’s leading new research area.

[Content of the Research Project]
We broadly have four parts in this research area (A01-A04) and will deepen each study and offer feedback to each other through collaboration.

Group A01 will focus on the impact of radionuclides on the atmosphere to elucidate the atmospheric circulation modeling of the fallout radionuclides, migration process, atmospheric deposition, diffusion process and the interaction of land surface.

Group A02 will focus on the effect of radionuclides on the ocean. They will study the distribution factor and condition of radioactive materials in sea and seafloor and also understand the migration and concentration of radionuclides in marine ecology.

Group A03 will be focusing on the effect of radionuclides on the land. They will find out the migration process of radionuclides associated with water and sediment and also the radioactive migration in terrestrial plants and ecosystem.

Group A04 will focus on the chemical forms of migrated radionuclides and the development of the measurement technology for various chemical forms.

[Expected Research Achievements and Scientific Significance]
We will launch a cross-sectional team, which consists of related but different study fields with geoenvironmental researchers as a core, to understand current contamination status and to construct a model for transfer and diffusion processes of radionuclides. Scientific insights and foundation for modeling which require long-term measures will be established through various interdisciplinary studies. With this interdisciplinary study on environmental transfer of radionuclides from the Fukushima Daiichi NPP Accident, we aim at strengthening academic levels of geoenvironmental sciences of our country, which in turn will contribute to the society.

[Key Words]
Fukushima Daiichi NPP Accident, Cs-137, Land, Ocean, Life, Atmospheric circulation, Entrainment

[Term of Project] FY2012-2016

[Budget Allocation] 923,800 Thousand Yen

[Homepage Address and Other Contact Information]
http://fsetr.suiri.tsukuba.ac.jp/