

## Research Center Project (in English)

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**Research center:** Earth-Life Science Institute (ELSI)

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### Project summary

· Briefly describe the general plan of the project.

#### 1. Research Objectives

The **Earth-Life Science Institute (ELSI)** aims to answer the fundamental question "**when and where did life originate and how did it evolve?**" This question, which originated with the Greek philosophers, has been one of the most important topics of natural science. We will focus our research on understanding the wide range of planetary processes and environments on the early Earth that may have been essential to the birth of life, and on their subsequent changes, with the main aim to study the origin and early evolution of life and persistent ecological systems in their geological context. We will use the enormous diversity of microbial biochemistries, physiologies, and ecologies as windows to identify how the biosphere has depended in detail on its planetary home from the past to the present, and to suggest the domains within chemistry and the planetary environments that are most likely to have been pivotal. We will approach the primordial environment of the Earth both through planetary measurement, theory, and modeling, and by using the many proxy environments available on the present Earth, ranging from deep-sea and sub-surface microbial ecosystems to extraterrestrial primitive asteroids. In addition, we will critically examine the universality of these processes, to determine the uniqueness of our planet, with implications for the search for extraterrestrial life, both in the solar system and beyond.

ELSI has been thoroughly interdisciplinary since its inception, integrating five areas in science that are essential for understanding the early stages of Earth and life. Addressing the challenges within these together will culminate in the ability to compare and more deeply understand emergent phenomena, which we call *comparative emergence*.

1. Geological sciences, including geology, geochemistry and geophysics of the early Earth, as the sciences that describe the environment in which life first originated, and which shaped, and in turn was shaped by, its further evolution.
2. Chemical sciences, including synthetic, computational, and systems chemistry, as the sciences of the unique physical medium that hosts living structure and dynamics.
3. Biological sciences, ranging from biochemistry and systems biology to environmental microbiology, and microbial ecology, as the sciences that both seek to understand the function and evolution of life, and that also contain our most important information about its deep connection to the detailed planetary context on Earth or possibly elsewhere.
4. Astronomical sciences covering scales from planets to galaxies, as the sciences that describe how the Earth was formed and what the surface environment of early Earth was like when life was born, and which explore how unique or common the Earth is in the galaxy and the possibility of life in other celestial bodies in our Solar systems and exoplanetary systems.
5. Broadly interdisciplinary input from a range of other scientific fields, from mathematics and physics all the way to computer science and cognitive science, to shed completely new light on the age-old question of what the nature of life is, and how that first appeared and then evolved.

Why these five areas? The most fundamental shift that we propose to make in studying the origin of

life is understanding that life is inherently a planetary process. It is the particular architecture and dynamics of a forming planet that not only hosts life, but also defines the framework within which living order forms and persists. The biological sciences, understood in this context, not only provide details about possible early life forms, and the history through which they became more complex and robust, but also principles to help understand in what ways life is a novel addition to a planet, and in what ways it is a continuation of planetary organization already present. Third, the life we know is inherently a chemical process. We need chemistry to understand how life's building blocks formed and how they first supported evolution, but for life to be chemical means much more. Chemistry is not only a science of techniques to produce and manipulate molecules, but a set of concepts explaining how simple rules give rise to complex organizations, because of the discrete and diverse character of atoms, bonds, and phases. Each of these three bodies of domain knowledge therefore carries some of the concepts essential to understanding life's origin and nature.

If there was any good agreement about roughly where and how life formed, those three areas taken together might be enough to produce more and more refined models of the co-evolution of life and environment, right from the appearance of the first living cells. However, currently we are still rather far from such a situation. The debate about how life may have formed continues to range over a huge spectrum of possible environments, together with a wide set of theories of which molecules combined how to produce self-sustaining reactions that were both robust enough to be preserved and flexible enough to admit increasing growth in complexity through early forms of evolution. As long as we don't really have a strong clue as to which ideas are correct, it is a good idea to step back from the immediate details, and to solicit ways of thinking from other areas in science and mathematics.

Recent astronomical observations suggest that more than 20% of solar type stars harbor Earth-size or super-Earth size planets in their habitable zones. These observations combined with theoretical modeling of planet formation will give important clues on how unique or common the Earth is within the galaxy. Discussions on habitable planets, which may have diverse surface environments, have led us to consider the possibility of life in the subsurface oceans of icy satellites in our Solar systems, in addition to that of life on exoplanets in habitable zones of other stars. These arguments will enable us to see our Earth and life on the Earth from a more general point of view. This is where the fourth area comes in.

The fifth area comes in, combining a range of broadly interdisciplinary sciences.

For example, in the last century some well-known physicists have moved into biology and thereby have triggered novel theoretical ways of thinking. In a similar fashion, it may well be that abstract modeling of self-sustaining processes, grounded in an understanding of chemical principles but capable of generalizing where appropriate, may teach us how to think on higher levels of abstraction about the origin of life. Computer science may have a unique importance for the problem of origin of life. More applied computation can support the analysis of systems such as chemical reaction networks at levels of complexity not previously possible, while the abstract understanding of algorithms may capture aspects of chemical and evolutionary function not normally recognized. The key to ELSI's interdisciplinary approach will be to tightly integrate both roles of computation. And finally, cognitive scientists with experience in pattern recognition and pattern generation and other cognitive processes may help in other ways: they may approach the interactive needs of the most primitive proto-cells in ways that biologists who are trained to work with current life forms may not easily stumble upon.

More specifically, here are the main research topics at ELSI, focused on the following questions:

#### **(A) Origin of the Earth**

- A1. How was the Earth formed?
- A2. How did the magma ocean phase connect early formation/differentiation to conditions when life emerged, including the essential element of water?
- A3. How has the Earth's structure, composition, and dynamics evolved through time?

#### **(B) Birth of Earth-Life system**

- B4. What was the state of the ocean and the atmosphere when life emerged?
- B5. How did the geological conditions of the early Earth influence the origin of life?
- B6. What was the nature of the first genetic systems employed in the "progenote"?

#### **(C) Evolution of Earth-Life system**

- C7. What were the major transitions in bioenergetic systems, what drove them, and how did they affect the spread of life?
- C8. How were ancient enzymes and genomes different from modern ones, and can we reconstruct models

of ancestral phenotypes?

C9. How did the thermal evolution of the solid Earth change the ecosystem?

#### **(D) Bioplanet in the Universe**

D10. How unique is our planet?

D11. How should we search for extraterrestrial life?

D11. What principles lead to life in a planetary context?

Our superiority in these studies is clear. We will study the unique environments on the early Earth by combining the research utilizing high-pressure/high-temperature experiments, theory of planet formation, and decoding the Earth's history, all of which are areas in which research at the Tokyo Institute of Technology (Tokyo Tech) is ahead of that at other places, nationally and internationally. In addition, Japanese scientists are also playing leading roles in molecular and evolutionary microbiology, in the study of wide-ranging microbial ecosystems including many in extreme environments such as hydrothermal vents, and crucially, in connecting the comparative analysis of microbial energetics to detailed geological contexts.

Moreover, we already have a rich tradition at Tokyo Tech in addressing many of these issues, based on unprecedented interdisciplinary research on Solid-Earth Science, Planetary Science, Geology, Materials Science, Environmental Biology, Molecular Biology, and Microbial Genome Science. Such collaborative research has been carried out by teams similar to ours since 2004 through the 21st century COE (Center of Excellence) Program and the Global COE Program. Based on our achievements in these programs, the research at ELSI will emphasize the roles of Earth's interior and the Universe in the origin and evolution of the Earth-life system. The main novel addition will be the even broader interdisciplinary connections in the fifth area listed above, for which we will make strong international connections with interdisciplinary groups elsewhere, such as the Program in Interdisciplinary Studies at the Institute for Advanced Study in Princeton.

## 2. Organization

The center is led by the director, Prof. Kei Hirose, who has the overall responsibility to create a world-leading research center. He will continue to recruit leading scientists from around the world and give them both clear roles and freedom in research. The center director makes the final decisions regarding the management of the institute, and appoints all the research and administrative staff members. The steering committee and the Director's office, in collaboration with the international advisory board will support and advise the director in the overall operation of the center, appointment and evaluation of each staff member.

ELSI has fifteen principal investigators, as of April 2017, including eight non-Japanese, one women, and three from the Satellite institutes (Ehime University, Institute for Advanced Study in Princeton & Harvard University). ELSI also has Associate Principle Investigators who have longer appointment more than five years. Young researchers at ELSI, called Research Scientists, have much freedom in research with loose connection to a specific group. Young researchers receive structured feedback and monitored throughout the year by mutually-agreed mentors. The research activity by research scientist will be evaluated annually. Based on such evaluation, the high achievers are given the incentive awards. Top scientists from various disciplines serve as ELSI fellows. Based on their expertise, they provide research guidance and advice to research groups and individual researchers.

Interdisciplinary research is promoted through extensive communications between the different groups. Piet Hut, Professor of Interdisciplinary Studies at the Institute for Advanced Study (Princeton), has built regular events such as daily coffee time, twice-a-week lunch talks, monthly ALL-ELSI meeting, and ELSI assembly presentations that stimulate broadly interdisciplinary interactions.

The operations and administration is led by the administrative director, Dr. Takashi Sakurai, who has rich experience in the institutional management and development at the National Astronomical Observatory of Japan, with the aid of Executive Administrative Director. Proper administrative officers of Tokyo Tech have been assigned to ELSI, providing the primary interface with existing administration offices of the university. Other administrators also have highly professional skills in research administration and English.

ELSI will have four Satellite Centers at Ehime University, University of Tokyo, the Institute for Advanced Study in Princeton, and Harvard University (Figure 10). We have also made strong connections with the Institute of Space and Astronomical Science (ISAS) of the Japan Aerospace Extrapolation Agency (JAXA), and the Japan Agency for Marine Science and Technology (JAMSTEC). These two agencies perform large-

scale investigations of extraterrestrial bodies and deep-sea hydrothermal systems, and their research targets are closely related to our scientific goals. In addition to these institutes, we have been collaborating with ten centers abroad on the basis of the ELSI Origins Network (EON) project funded by the John Templeton Foundation, with which we hire joint postdocs who spend half time at ELSI and the other half in the overseas centers. Such collaboration through joint postdocs is an important part of ELSI's mission to become an international hub of research interactions.

#### <Major changes from initial project plan:>

- ELSI has strategically enhanced its research organization. ELSI appointed new PIs with strong expertise in Biology and Chemistry. By setting up the fourth Satellite Center at the University of Tokyo, ELSI will further reinforce Earth and Planetary Sciences. We set up dialogue-based forums to discuss strategic development goals and accelerate interdisciplinary collaboration.
- By acquiring the large research fund from the John Templeton Foundation, ELSI launched the ELSI Origins Network (EON) project, which has expanded ELSI's international network and attracted a diverse collection of young talents in the Origin of Life studies.
- Following discussions over the institutional development described above, ELSI has conceptualized the idea of a new research domain. ELSI aims to crystallize this idea of "Comparative Emergence" in the coming five years.
- ELSI has introduced a mentoring system to ensure structured feedback to early-career researchers.
- ELSI has started accepting PhD students and is eager to recruit more prospective PhD students.

#### <Mission statement and/or center's identity>

- Briefly and clearly describe the mission statement and/or the project's identity as WPI center.

So far, discussions about the origin of life on Earth have been mostly limited to the biochemistry of proto-life forms. While the Earth environment has been described as a "cradle of life", the image of a "cradle" points to a supporting background role, rather than a dynamic interplay. In ELSI, we want to radically broaden these discussions by focusing equally strongly on both sides of Earth and Life. For one thing, life is preserved through a continuous exchange of matter and energy with the surrounding environment. For another, it is a two-way interaction: as soon as life forms are present, they start to influence the environment, just as the environment is influencing life. Our basic outlook is reflected in the name of our proposed center: ELSI stands for Earth-Life Science Institute, in which Earth sciences and Life sciences will be equally represented.

In addition, we will replace the biology question of the "origin of life" with the more relevant interdisciplinary question regarding the "birth of a persistent ecological system." An important goal in our research will be to clarify the initial ecological system that allowed a stable and persistent existence of life even under the various harsh and violent changes of the environment at the beginning of the Earth's history.

And while we will study life in the context of the early Earth environment, similarly we will also study how the Earth itself was formed and how its conditions changed, inside the Earth as well as on the surface. In the course of these studies, we will critically examine the universality and uniqueness of our planet that gave birth to life as we know it, with implications for the search for extraterrestrial life in both solar and extra-solar systems.

We will perform our research through cutting-edge lab experiments, computer simulations, and field observations. We may also need to develop wider pictures of metabolism and self-reproduction on more abstract meta levels through a broadly interdisciplinary approach. How such abstract models are then implemented on molecular levels may differ between life on Earth and elsewhere.

In contrast to NASA's Astrobiology Institute (NAI) whose research topics are broadly similar to ours, we emphasize the role of the Earth as a whole in the origin and evolution of life. Most importantly, ELSI will not be a virtual institute like NAI. People from different fields will gather together at ELSI to make it a foremost interdisciplinary research institute. We will promote internal communications through a series of daily, weekly, and monthly events, following the Program for Interdisciplinary Studies at the Institute for

Advanced Study (IAS) in Princeton as a model. This IAS program has been a satellite center for ELSI.

The success of ELSI will depend strongly on its research environment, and the recruitment of good scientists. We have strongly encouraged interdisciplinary research within ELSI, which attracts a wide variety of top scientists to visit ELSI to interact with members there and also with each other. We do not want to define job specifications too strongly beforehand. Rather, we prefer to attract top scientists first, and then to finetune the research program around their skills and interests. In addition to promoting internal communications, the center director is responsible for providing the best research environment. A very efficient research-oriented secretary system has been created through evaluation and education of administrators.

ELSI is now playing a strong role as a communication center. We have promoted interdisciplinary connections between researchers internationally and nationally. In addition, we combine our research with outreach and education. The on-going Hayabusa-2 mission as well as the future plan called MMX mission to Mars moons, questions about the formation of Earth and the origin of life, and extraterrestrial life are of strong interest to the general public, and thus perfect for outreach. As for education, we will start an international graduate program with top-level students including many from abroad. These activities help not only ELSI but also its host, Tokyo Tech, to further increase both its international and domestic visibility.

## 1. Research fields

- Specifying the inter-disciplinary field(s) to which the project may be closely related.
- Describe the importance of the proposed research, including domestic and international R&D trends in the field and Japan's advantages.
- If centers in similar fields already exist in Japan or overseas, please list them.

### **Interdisciplinary Research on Solid-Earth Science, Planetary Science, Geology, Environmental Microbiology, Microbial Genome Science, Systems Chemistry, Complex Systems Science, and Comparative Emergence**

We will promote integrated research in fields related to the formation of the Earth in the early solar system, the environment and the creation of life on the early Earth, and the co-evolution of the Earth-Life system, using the keyword "early Earth". Through the study of Earth, we will clarify both universal and unique aspects of the Earth, from which life emerged and evolved, and we will predict the presence or absence of life on other planets. In order to immediately apply our research results to search for extraterrestrial life, we will work in close cooperation with space exploration missions and astronomical observation teams. To overcome the frequently-claimed problem of an "n = 1" sample for both Earth and Life, we will apply the range of comparative methods across physical and biological sciences to understand common aspects of the emergence of novelty among the many subsystems that make up each domain. We refer to this application of modern comparative methods to a systematic study of emergence as a natural phenomenon in its own right using the keyword "comparative emergence".

#### **Importance and trend of the research field**

The life science and Earth science should be linked, simply because life is a phenomenon that can exist only through the exchange of energies and matter with the surrounding environment. We will therefore integrate research on the Earth and life, and explore "how our life can originate and continue on this planet" through a detailed study focused on the early Earth. This is one of the most important questions that natural science, beginning with Greek philosophy, has asked until this modern age. It is amazing and fascinating that so much progress has been made during the last 20 years, in related fields, on a question that has been at the heart of science for 2700 years. Four trends will be described in the following sections.

#### **1. Understanding the Earth**

Recently, rapid progress has been made in analyzing the deepest parts of the Earth, and we now have a detailed image of the Earth's interior, including the core of the Earth. One of the major factors in this progress has been a drastic advancement in ultrahigh pressure experiment techniques by Hirose, Center Director, and Irifune, a PI based at the Ehime Satellite Center. Fifteen years ago, most experiments covered a depth of only 2000 km, but currently experiments studying the center of the Earth, 6371 km deep, are being routinely conducted. Large volume high pressure experiments can now be performed up

to conditions of the deep mantle in Irifune's lab, using a technique that strongly complements and supports the technology in Hirose's lab. As a result of these developments, Hirose et al. discovered that the lowermost mantle is composed of a previously unknown mineral phase, post-perovskite. Furthermore, Hirose et al. have analyzed crystal structures of the inner core at the center of the Earth. As a result, the actual state of the Earth's core, which so far had been a topic of speculation, is now a regular subject of experimentation in ELSI laboratories. These are great accomplishments achieved in Japan. The high pressure experimental achievements of Hirose and Irifune have raised the global visibility and importance of frontier geoscience in Japan, which has led to growth in international collaborations and advances in our understanding of Earth's evolution.

Most of the past ultrahigh pressure experiments were conducted to understand the "present Earth," however, the direction of research enabled by recent developments now allows us to directly target "the evolution of the Earth" and "**the early Earth.**" For example, PI Hernlund and his team used the discovery of post-perovskite, combined with seismic imaging, to constrain the rate of cooling of Earth's core, a critical parameter controlling Earth's long term evolution and dynamics. The high cooling rate of the core implied by this result led Hernlund to propose the "Basal Magma Ocean" hypothesis, which was experimentally confirmed by experiments performed in Hirose's lab. PI Helffrich recently used seismic imaging to show layering in the outermost core of the Earth which is connected to chemical exchanges between the core and mantle that are simulated at high pressure by Hirose and Irifune. And a major discovery has recently been made in Hirose's lab showing that the core crystallizes  $\text{SiO}_2$ , providing an explanation for how Earth could have maintained a geomagnetic field more than 3.5 billion years, as suggested by paleomagnetic evidence. At the same time, PI Kirschvink and his group have developed micro-magnetometer techniques that permit us to measure Earth's remnant magnetic field recorded in zircon crystals older than 4 billion years, before the rock record. Thus we are able to extend our evolution constraints back to Earth's formation period 4.5 billion years ago, where we can connect with unique constraints from planet formation models like those pioneered by PI Ida. From this work, it is apparent that the extensive differentiation of the Earth due to magma oceans is a major factor controlling the subsequent evolution of the Earth, which in turn determines the conditions of the surface environment.

Complementing these discoveries, the progress of research on geology and geochemistry of the early Earth environment is remarkable. As a result, on a macro and long-term time scale, it is becoming clear that Life and Earth evolved together. In the 1980's, the Precambrian Paleontology Research Group led by Bill Schopf found many bacterial fossils in Precambrian rocks older than 1 billion years ago. This revealed that life was active on the early Earth. Unfortunately, it was impossible to classify the fossil bacteria based on their simple forms, and it was unknown "what functions and metabolisms were active on the early Earth." After that, the geochemical bio-indicators such as stable isotope ratios of bio-essential elements were established, and certain physiological natures and metabolisms could be continuously read off the geological records. Currently, the biogeochemical cycle of C, N, S, and Fe, etc. can be traced back to 3.8 billion years ago. Furthermore, this research on geochemistry is reaching a level that produces quantitative estimates of the chemical environment on the early Earth, including the atmospheric composition and redox status of the oceans. The "decoding whole-Earth history" project led by Kumazawa and Maruyama, Institute PI, pioneered this research in Japan since 1995. Then, internationally, the Agouron Institute started their scientific drilling project in the Kalahari Desert in South Africa (PI, Kirschvink), followed by the NASA Astrobiology Institute and continental drilling programs of France and Australia, etc. Research programs by Tokyo Institute of Technology COE/G-COE programs also played a role in the research of the evolution of the Earth.

The results of this research uncovered unexpected aspects of atmospheric evolution, such as the Great Oxidation Event, and climate changes, such as Snowball Earth, found by Kirschvink, an Institute PI, implying an important relationship between environmental changes and the evolution of life. The ultimate causes for these environmental changes have not yet been identified; however, changes of the solid Earth (rapid continental growth, increase in sedimentary rocks, intense volcanic activities and geomagnetic field intensity changes), sudden biological evolution of oxygen-releasing photosynthesis, and the impact from galactic events (increase in cosmic rays on Earth), have been actively discussed. A number of new concepts have originated from interdisciplinary research by Tokyo Institute of Technology's G-COE program. To determine the origin and evolution of life on Earth, it is time to pay close attention to the relationship between the thermal evolution of the Earth including its deep mantle and core and long-term changes in the Earth-Life system.

## **2. Earth-Life Geobiology and Comparative Microbial Genomics**

Microorganisms seem especially good at adapting to extreme physical and chemical conditions, and

the diversity of these conditions is in turn connected to the development of the vast diversity of life on the planet. Furthermore, the existence of microorganisms in apparently very extreme environments motivates the idea that extraterrestrial life may have a capacity to thrive in a wide array of chemical environments. However, the relationships between physical-chemical conditions and microbial evolution have not been established. Nor have the time scales and magnitudes of microbial driven global chemical change been clearly delineated. Connecting biological evolution to planetary evolution is a key goal of ELSI, and in the scientific community the recognition of the importance of this connection led to the establishment of such concepts as “biogeochemistry”, “geomicrobiology”, and also broadly, “geobiology”.

To understand the collective relationships between biological-abiotic-geological interactions during long and very evolutionarily significant time scales requires diversity of intellectual breadth and at the same time substantial focus. This intellectual breadth has now been achieved in the unique ELSI environment. For example, ELSI researchers investigate microbial biogeochemical interactions and their evolution from a number of angles and also using distinct yet integrate-able study systems including: hyperthermophilic viruses, the bioenergetics of archaea and bacteria, protein catalyst evolution and its geological fingerprint in the rock record, the evolution of major bioenergetics transitions such as photosynthesis, microbial biomineralization processes, advanced next generation genomics analyses, and cutting edge single cell analytical techniques to enumerate cellular activities as they exist in natural environments.

The establishment of a new field of cellular ecology based around the perspective of individuals has also shifted research focus at ELSI and worldwide. Now, it is possible to construct an understanding of microbial ecology directly from thousands of individual observations; in the future, these observations will turn into millions, extending the perspective of the individual throughout microbial ecosystems. These developments assist in interpreting how and why genomically identical individuals within populations vary significantly between each other, and how these differences might be closely linked to the geologically determined physico-chemical environment. This perspective on cellular individuality connects and supplies contrast directly to other ELSI research on the “progenote” – which references a time in biological evolution when individuality did not exist in the current form.

In addition to the ability to perceive ecology from the individual cell perspective, microbial genome and metagenome sciences are keys to understand the early and modern ecosystems and to extract general principles from the great complexity of ecosystem formation and behavior. Still, the unknown diversity of microbial genomes and their physiologies remain vast, however rapid development of next-generation sequencers and data analysis methods enable us to obtain, extract and interpret enormous amount of data and information, expanding our knowledge at unprecedented rates. Using these approaches new perspectives on the evolution of bioenergetics capacities such as photosynthesis and hydrogen oxidation can be gained. These capabilities clearly establish genome sciences as a key strength within ELSI.

### **3. Messy Chemistry: from components to system-studies of the Origin of Life**

While a precise definition of life is yet to be rendered, it is understood that a living organism is not a mere collection of molecules, but an extensive complex dynamic network of interlinking processes. It is therefore reasonable in the search for the origin of life to give attention to prebiotically plausible chemical systems that could have sustained life-like processes. As it stands a number of experiments simulating early earth conditions, such as Miller-Urey experiment (Miller, 1953), hydrogen cyanide polymerization (Matthews and Minard, 2006), formose reaction (Breslow, 1959), have been shown to be complex chemical systems invoking a large number of reaction mechanisms and yielding a vast array of products. We describe such systems as “messy chemistry”. While these systems are usually reported as sources of biological building blocks, within them processes leading to the synthesis of amino-acids, nucleobases and carbohydrates are by far not the predominant ones. In fact, the major product is usually the mixture of intractable structurally complex polymers referred to as “tar” or “asphalt”. How did such undesired processes get suppressed in the prebiotic world without enzymes to favor relevant ones? Alternatively, did the “tar” play an important role in the process of chemical evolution?

Conditions of the earth and specific geological phenomena are likely to have shaped the prebiotic chemical systems. Of fundamental importance to all synthetic chemical systems are free-energy sources, among which natural nuclear reactors combining ionizing radiation with wet-dry cycling are one possibility, and organized electrochemical potentials at chimney structures in hydrothermal vents are another. These relatively recently-investigated sources could have acted independently of or in parallel with other long-investigated energy sources including oxidation/reduction potential from mixed non-equilibrium fluids, and far-from equilibrium chemistry in space producing organized molecules that could be delivered to Earth. Active areas of research at ELSI in natural-environment modeling will emphasize possibilities for nuclear geysers in the Hadean (more ancient than those preserved in known geological formations), utilizing Tokyo

Tech's unique irradiation facilities, and hydrothermal vent experiments and laboratory models focused on the reduction of CO<sub>2</sub> to form organics that could plausibly have existed on prebiotic Earth. Given the centrality of redox reactions in contemporary metabolism, the study of geological triggers for this type of chemistry is of particularly importance.

Complex systems chemistry is a relatively young field, basic tenets of which are still being formulated without the added constraint of prebiotic plausibility. One group of approaches that guides ELSI's research program is *artificial chemistry*, a computational field wherein chemical reactions are computer simulated, yielding insight on emergent phenomena, self-organization and evolution in general. Our inquiries will focus in-depth on intermolecular force driven self-organization and selection, both *in silico* and in the laboratory. The experimental studies within the framework will concentrate on chemical systems that are not necessarily prebiotic but discernable by the established analytical techniques.

An important parallel contribution to ELSI's research in systems chemistry comes from advances in computational methods for handling the combinatorics of both molecular state spaces and reaction systems. Partly these advances come from increases in computing power in the last decade, and partly they draw from advances in the abstractions with which reactions can be represented and analyzed. The widespread use of abstract molecule representations such as SMILES and INCHI (Weininger and Weininger, 1989; IUPAC 2016) have enabled database approaches and context-sensitive representations of reactions, but these systems have also revealed weaknesses in the molecular representation that render them insufficient for unlimited extension. Recent improvements in the representations of molecules and reaction abstractions in terms of graphs and graph-rewrite rules, combined with computational advances in costly algorithms such as graph-isomorphism search and integer linear programming, now enable the automated generation and characterization of networks that would have been prohibitive even ten years ago. New tools, introduced by ELSI collaborators, network affiliates, and even postdoctoral fellows, include the molecular structure calculator MOLGEN ([www.molgen.de/](http://www.molgen.de/)), and the graph-grammar reaction-modeling framework MedØIDatschgerl. ([cheminf.imada.sdu.dk/mod/](http://cheminf.imada.sdu.dk/mod/)).

In parallel with discrete methods to represent molecules and reaction systems, advances in molecular dynamics, density functional theory, and *ab initio* methods (propelled significantly by their use in the pharmaceutical industry) have made possible the quantitative modeling of enzyme-substrate fit and reaction transition states, to a degree that can be calibrated against experiment and used to predict isotope effects or consequences of mutation or atomic substitutions. With these we can pursue the reconstruction of ancient enzymes and deduce the aspects of molecular phenotype that were essential to their evolution.

Complex systems methods relevant to understanding the emergence of order in driven systems also include general theory of pattern-formation and robustness from non-equilibrium stochastic processes. At ELSI we will apply these, not only to traditional problems in reaction-diffusion theory where they remain relevant and challenging, but also to new domains such as the topologically and computationally complex systems known as chemical reaction networks, following the pioneering work of Feinberg, Horn, and Jackson (Horn and Jackson, 1972; Feinberg, 1987). Other important influences on ELSI complex systems studies include a fully modern understanding of evolutionary dynamics, across levels ranging from molecules to ecosystems, and even theories that seek to abstract the essence of cognitive capabilities, where we collaborate with innovative centers such as Araya Brain Imaging.

Messy chemistry is an interdisciplinary approach combining the expertise of earth science, complex system physics, organic and biochemistry. Consequently, ELSI is uniquely positioned to apply messy chemistry to the origins of life studies.

#### **4. Discovery of "Earth-like" exo-planets**

Since 1995 when extra-solar planets were first found, the number of planets newly discovered has increased drastically; as of 2016, 3500 extra-solar planets have been confirmed. Many terrestrial planets ("super-Earths" and "Earths") have been discovered beyond the solar system in the last decade, and the minimum detectable planetary sizes have reached down to the Earth's size. The most recent observations and theoretical models suggest that more than 20% of solar-type stars have super-Earths or Earths in their habitable zones, stimulating discussions about extraterrestrial life within the field of astronomy. From these diverse and ubiquitous super-Earths/Earths, we can understand our Earth more deeply.

At ELSI, planet formation theory has been developed to discuss formation of both our Solar system and exoplanetary systems. ELSI is now one of world-leading centers on planet formation theory. An Institute PI, Shigeru Ida, developed a planet population model that enables us to directly compare between the theory and exoplanet observations, which have been significantly referred to by many exoplanet survey projects in the world. N-body simulation of planet accretion is also a strong point of ELSI. Now, cosmochemical data are also combined to the theoretical simulations, in addition to astronomical

observation data of protoplanetary disks and exoplanets.

In a parallel development, the discovery of past water traces on Mars and the observations that strongly suggest the existence of internal oceans in Europa (a satellite of Jupiter) and Enceladus (a satellite of Saturn), have given us great expectations that there might be other celestial bodies in the solar system that harbor life. Formation model of icy satellites has been also intensively investigated by ELSI researchers.

Thus, it might be becoming possible to find (signatures of) life on extraterrestrial celestial bodies. Using current or future astronomical observation, we can begin to look for biosignatures of extraterrestrial life. The major idea is to detect atmospheric components of possible biological origins, such as ozone or methane, by direct spectroscopic observation of extra-solar planets. Such an observation is one of the highlights of next-generation large ground-based telescopes such as TMT (Thirty Meter Telescope) and E-ELT (European Extremely Large Telescope) planned by international consortiums. On the other hand, ALMA (Atacama Large Millimeter/submillimeter Array) radio telescope developed by international collaboration has already started observations and is discovering complex organic matter in interstellar molecular clouds and revealing the detailed structure of protoplanetary disks around young stars, where planets are forming.

The search for extraterrestrial life includes *in situ* analysis or sample return by space missions in addition to the remote sensing by telescope observations. While many space missions have been targeted to *in situ* surveys of surface of Mars, sample return missions such as “Hayabusa-2” by JAXA are also promising. In samples from a primitive C-type asteroid (Ryugu) that will be obtained by Hayabusa-2, water and organic matter should be found. JAXA is also planning a sample return mission to a Martian satellite (Phobos or Deimos) called MMX (Martian Moons eXplorer), which may be launched in 2024. MMX will give an important clue not only to the origin of Martian satellites but also primitive Martian surface environments, because it is expected that the samples also include debris generated by early impacts to Mars. ELSI researchers have been committing to science goal discussions of MMX, and ELSI is expected to play an important role in MMX mission plan.

As just described, science missions searching for extraterrestrial life have already started, and atmospheres of extra-solar Earth-like planets will be investigated through spectroscopic observation within next 10 years. Thus, the understanding of the universality and uniqueness of our Earth, and the presence or absence of biological activity on extraterrestrial celestial bodies will dramatically advance. In this way, Earth and planetary sciences will be revolutionized, upon finding habitable celestial bodies beyond our current imagination. For such observations, we need to establish a new field of “Bio-planetology” that will predict the conditions of planets (or other celestial bodies) allowing existence of life and what observation methods should be used for finding them. This should be an urgent issue for earth and planetary sciences and astronomy. In 2015, Japan AstroBiology Center (ABC) was founded. Its main objectives are to develop instruments for TMT and promote on-going extra-solar planet search programs. ELSI researchers have been involved as board members of ABC. Close corporation between ELSI and ABC is expected.

### List of centers in similar research fields

International:

- NASA Astrobiology Institute (NAI)
- SETI (Search for Extraterrestrial Intelligence) Institute
- Harvard Origins of Life Initiative
- Heidelberg Initiative for the Origins of Life (HIFOL)
- Centre for Earth Evolution and Dynamics (CEED)
- Institut de Physique du Globe de Paris (IPGP)
- Centro de Astrobiología (CAB), CSIC-INTA
- Simons Collaboration on the Origins of Life (SCOL)
- Center for Chemical Evolution (CCE)
- Continental drilling programs (France, South Africa, Europe), Deep-sea drilling programs (ODP, etc.)

Domestic:

- Japan Agency for Marine-Earth Science and Technology (JAMSTEC)
- Institute of Space and Astronautical Science/Japan Aerospace Exploration Agency (ISAS/JAXA)
- AstroBiology Center (ABC), National Institutes of Natural Sciences (NINS)

### Japanese expertise

In this institute, we “recreate the Earth” through ultrahigh pressure experiments and simulations based on planet formation theory. We increase our understanding of the origin and early evolution of the Earth-Life system through geological and microbiological research, and study the universality of life-hosting planets through generalizing from the case of the Earth. Among these, ultrahigh pressure experiments

and planet formation theory are, without a doubt, world-renowned specialties of the Japanese in the fields of earth and planetary sciences. In the ultrahigh pressure experiments, the multi-anvil apparatus and diamond-anvil cell apparatus are the two major high-pressure instruments that are most widely used. The former apparatus was mainly developed by Naoto Kawai in Osaka University in the 1960's. The apparatus itself and experiment techniques have been exported worldwide from Japan. The person at the leading edge of developing these techniques is Irifune, an Institute PI. The latter apparatus has the disadvantage that microscopic samples are used; however, it has become a major apparatus for high-pressure earth science with the advent of radiation light facilities. Only the group led by Hirose, the Institute director, can realize the ultrahigh pressure and high temperature environment at the center of the Earth. Both groups, led by Irifune and Hirose, have achieved great results based on their world-class ultrahigh pressure experiment techniques, and the superiority of those results will certainly continue for the next 5 years. In addition, particle beams are required to analyze microscopic samples under high pressure. Having the world's most advanced high pressure sample analysis facilities, such as the world's largest facility for synchrotron radiation, SPring-8, and the Japan Proton Accelerator Research Complex, J-PARC, forms part of Japan's superiority.

Equally leading internationally, the classical standard model of planet formation was established from "Kyoto model" and Safronov model in the 1980's. Currently Ida's group in the Tokyo Institute of Technology (an Institute PI) has taken over, and a new "Tokyo Tech model" is being established. This process is closely connected with the development of large scale computer systems and comprehensively synthesizing multi-layered processes of planet formation. Makino, an ELSI Fellow, has contributed greatly to the development of the world's fastest super computer by a unique approach of integrating the development of hardware, algorithms, and software and scientific research, and his expertise will be invaluable.

In the 1990's, a project on "decoding the whole Earth history" was promoted mainly by Maruyama, an Institute PI. In this project, ahead of the inception of the encoding the evolution of life on the early Earth by the NASA Astrobiology Institute, much progress was made in collecting, encoding, and analyzing rocks from the early Earth worldwide. Rock samples collected from all over the world reached a total of over 165000 samples. These samples are stored at the Tokyo Institute of Technology and made available for collaborative research all around the world. Collecting rocks in consideration of the changes in the solid Earth is an exclusive part of this project.

For deep-sea hydrothermal exploration, Japan has the best capability in the world, led by the Japan Agency for Marine-Earth Science and Technology. Takai, an ELSI Fellow, et al. have initiated geomicrobiology of the deep-sea hydrothermal systems and have provided basic principles of interaction between the geo- and life-systems through more than 10 years of exploration by his group, utilizing world-class, large-scale research facilities.

While Europe and the U.S. lead the way regarding the observation of extra-solar planets in the universe, Japan has also achieved many essential results, such as sample return missions from asteroids via Hayabusa and Hayabusa-2 by JAXA and direct imaging of extra-solar planets using the Subaru Telescope. Another sample return mission to a Martian satellite (Phobos or Deimos) is also planned by JAXA.

In addition to the expertise of each individual researcher, the collective research done in the "project on decoding the Earth evolution", "Tokyo Institute of Technology COE project: the Earth" and "Tokyo Institute of Technology Global COE Project: From the Earth to Earths", provided interdisciplinary integrated research by geoscientists, planetary scientists, and life scientists. These research projects, starting 25 years ago, have firmly established Japan's leading role in these fields, internationally.

### **International appeal of ELSI**

ELSI has quickly become a key place for scientists to get together and develop new ideas. International appeal of ELSI can be distilled to two major points: 1) ELSI addresses fundamental questions to understand the origin and evolution of the Earth and life with equal focus on the Earth/Astronomical Sciences and Life/Chemical Sciences and 2) ELSI transformed vision into reality by establishing such interdisciplinary research institute as a physical entity. The unique features and the global status of international collaborative research centers are described in more detail below.

Recent decades witnessed increased international activities in fields such as Astrobiology, exoplanet observation, and investigations into microbial ecosystems in diverse and extreme environments. There is, however, little concerted effort by any other single institute except ELSI to make such a detailed collaborative effort to address the most ambitious questions of Earth and life sciences: the origin of Earth (planets) and the origin(s) of life. ELSI's interdisciplinary approach to these questions has been extremely successful in raising a very high international profile in just several years.

ELSI's international appeal is evident in the involvement of other institutions in international projects instigated by ELSI. ELSI was launched with its international network that consisted of three Satellite Centers, two of which located in overseas, and many overseas institute in cooperation. This global network was substantially enhanced through the ELSI Origins Network (EON). EON has founded a network of "affiliated centers" around the world, each of which shares a postdoc with ELSI who works on a joint project. These centers include groups in the US (at Emory university, Rutgers university, Caltech, UC San Diego, NASA Goddard and NASA Ames), Europe (at University of Southern Denmark and Institut des Systèmes Intelligents et de Robotique in Paris) and the UK (at Cambridge university).

It is obvious that interest in the origin and evolution of Earth and life is common among humankind in all ages and places. The possible existence of life on Mars and the icy moons Europa and Enceladus with potential internal oceans has been extensively discussed as a near future target for space exploration. Recently, a large number of extra-solar planets have been found, and some of them may have oceans like Earth. In this age when the existence of life in the universe is beginning to be scientifically discussed, we face an increasing importance of understanding the origin of the Earth, from which life has grown. The "early Earth" that we focus on, is an almost untouched field so far, waiting for the experimental and numerical techniques that we plan to use and are using today. As there is little direct physical evidence, research on the early Earth is a great challenge for geology and life science. It is clear that the early Earth and early Life followed a path of joined evolution. ELSI, as an international institute that researches on such unresolved important fields has attracted the eyes of the world.

What has established ELSI as an international hub among these in a short time is the fact that ELSI is an institute built in the university campus whereas others are mostly virtual organizations where researchers in different fields do their research separately in their own institutes. Researchers in different fields gather and interact at ELSI, and this face-to-face collaboration has destroyed the barriers that exist between research fields and cultures and is succeeding in integrating disciplines. As a result, the roles of the solid Earth and the universe in influencing the origin and evolution of life have been receiving growing attention as key concepts. This unique and increasingly globally recognized "ELSI brand" of Earth-Life science will continue to spur a wide range of interests and to advance research on the origin and evolution of the Earth and life, highlighting ELSI as a pioneer institute. In the next phase of the institute, we expect continued and even more dramatic international visibility and appeal.

## 2. Research objectives

- Describe in a clear and easy-to-understand manner the research objectives that the project seeks to achieve by the end of the grant period. In describing the objectives, the following should be articulated in an easily understandable manner: What kind of research do you plan to implement by fusing various fields within the environmental domain? In the process, what world-level scientific issues are sought to be resolved? What is the expected impact of the scientific advances to be achieved on society in the future?
- Describe concretely the research plan to achieve these objectives.

We focus on **the early Earth** when life emerged, and will answer the following scientific questions: (A) How was the Earth formed within the solar system? (B) How was the earth's first ecosystem established, and (C) How can the earth and life evolve after the first state. Through the study of the Earth, we clarify universality and uniqueness of the planet Earth harboring life. Further, we utilize the outcomes of the research (D) to provide guidance for the search for life on other planets and moons. Each of those themes is performed under an interdisciplinary fusion of different fields. Each question to be solved is discussed in detail below.

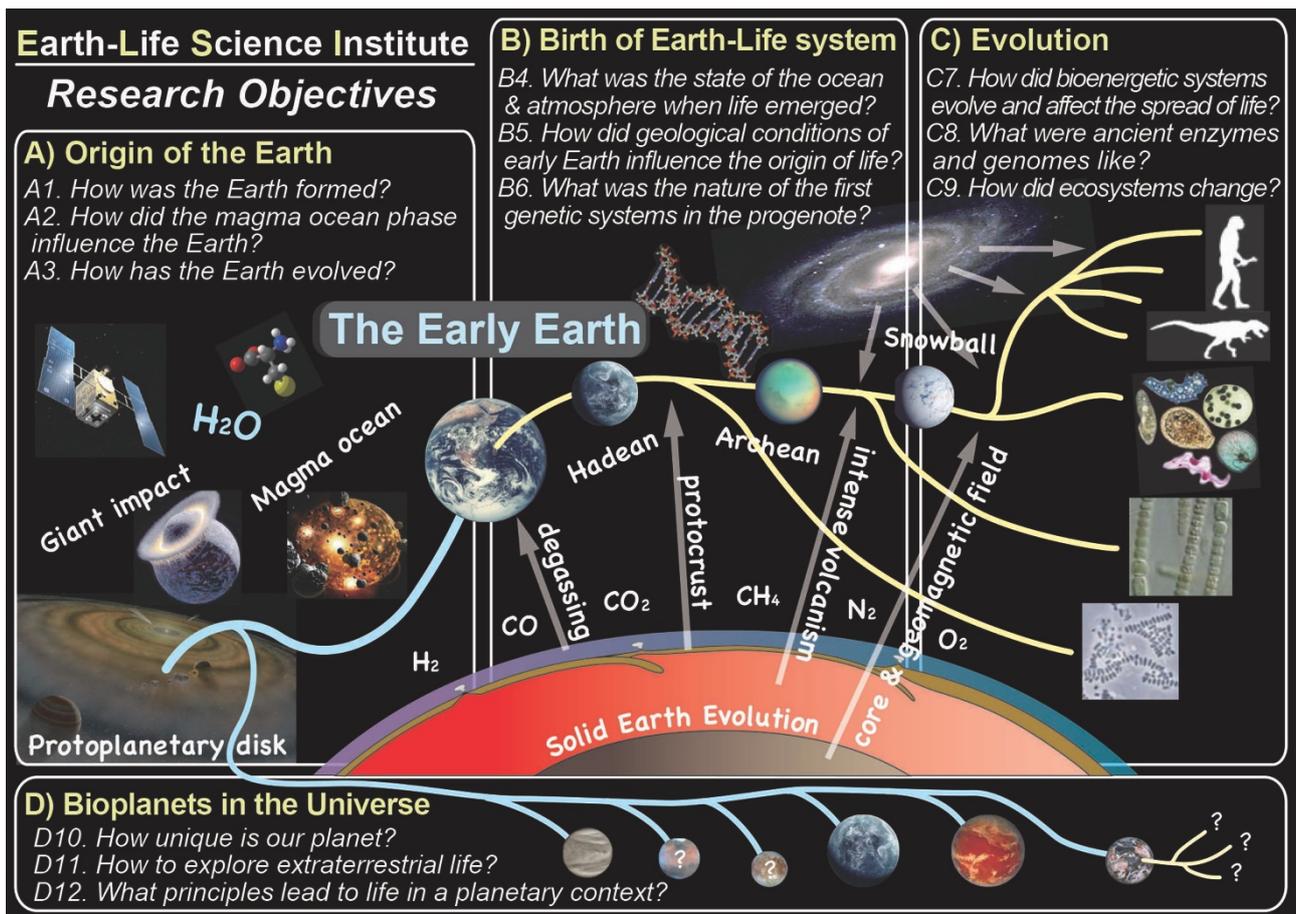


Figure 1. Summary of research objectives.

### A) Origin of the Earth

The main goal of our study is to understand how the planet Earth was formed and harbored life. It is critical to determine the original state of the Earth from the core, through mantle and crust, to the ocean and the atmosphere. First, we aim to understand (1) how the earth was formed in the solar system, examining the theoretical model from the viewpoint of the chemical composition of the Earth. (2) Breaking through the conventional idea of habitable zone (i.e. just presence of liquid water), we will find out factors which determined the appropriate level of ocean water on the Earth. And finally, (3) we experimentally reproduce material differentiation of the early Earth before and after the birth of life.

#### A1. How was the Earth formed?

The classical standard planet formation model was built from Safronov and Kyoto models in the 1970-80's to explain planetary configuration in the solar system. However, recent findings of diverse extra-solar planetary systems show that the classical model cannot be applied to the extra-solar planetary systems. We need to take into account many processes that were missing in the classical model to rebuild the planet formation theory, in order to explain both our solar system and diverse extra-solar planetary systems consistently. On the basis of the renewed planet formation model, we discuss delivery of volatile elements such as water and organic molecules that are essential for life. Presence of liquid water conventionally has been considered as one of the conditions for habitable planets, and the range of orbital radii in which liquid water can exist is called a habitable zone. Coexistence of ocean and land could also be a condition for a planet for life to emerge. However, the factors that determine the amount of water on a planet have not been clarified yet. Furthermore, we verify our theoretical models by clarifying the chemical composition of the bulk Earth and by determining the composition of the present core and lower mantle of the Earth on the basis of super-high-pressure experiments.

#### A2. How did the "magma ocean" phase connect early formation/differentiation to conditions when life emerged, including the essential element of water?

Terrestrial planets and moons are thought to form in an environment characterized by energetic accretion and extensive melting events called "magma oceans" that processed material delivered to the

growing planet and facilitated its differentiation into core, mantle, crust, ocean, and atmosphere. Magma ocean studies are therefore of critical importance to understand the birth of terrestrial planets and moons, and is a key bridge between research fields concerned with planetary accretion (A1) and subsequent evolution (A3).

### **A3. How has the Earth's structure, composition, and dynamics evolved through time?**

As the magma ocean was formed and solidified, the earth materials were differentiated into the core, the mantle, the crust, the ocean, and the atmosphere. Such material differentiation at the beginning of the Earth determined the subsequent mantle dynamics and thermal evolution of the Earth. Through volcanic activity, continental growth, and magnetic field formation, it should have had a significant influence on changes of the surface environment and the evolution of life. Surface conditions including that of the atmosphere couple influences ranging from the geomagnetic field generated in the deep earth out potentially to the scales of galactic structure. We investigate such a material differentiation by high-pressure experiment and computer simulation.

## **B) Birth of Earth-Life system**

In 1977, Woese and Fox proposed the concept of the progenote to refer to a period of biological evolution in which vertical inheritance was not yet the dominant form of information transfer. Thus, before phylogenetically distinct lineages emerged, a genetically co-interacting community existed out of which emerged what we now perceive as the three domains of life. This recognition leads to the notion that the so-called "origins of life" should be discussed as entirely different phenomena from the emergence of the most ancient living ecosystem of our ultimate ancestors. We focus on the first Earth-Life system including the atmosphere, the ocean, the rocks, and the biological community that co-evolved finally into the progenote and subsequently life as we know it. Our goal is to understand when, where, and how, the Earth-Life system was established. In ELSI, we will try to solve the following questions.

### **B4. What was the state of the ocean and the atmosphere when life emerged?**

What was the composition of the initial atmosphere, the ocean and the crust at the time of the birth of life? It is still largely an unsolved scientific question. We will build a verifiable model for the first ocean and atmosphere by 1) a forward approach based on the high-temperature experiments and theoretical simulations of A1 to A3, and 2) a reverse approach from the geological record. With the technical development of geochemical tracers, we will decode the chemistry of the early ocean and the atmosphere from rock records dating back to 4 billion years ago, and we will test the theoretical model thoroughly.

### **B5. How did the geological conditions of the early Earth influence the origin of life?**

The elucidation of the origin of life is a complex multi-layered undertaking. The solution requires the discovery of chemical reaction network in the context of geophysical constraints capable of supporting the emergence of life-like processes. On the one hand we explore the chemistry triggered by naturally occurring energy sources, such as nuclear geysers and geologically sustained electrochemical potentials provided by the hydrothermal vents. On the other, we make use of abstract computational methodology, artificial chemistry, to understand the dynamics and the emergent properties of complex system. Concentrating on function rather than structure, we investigate the enzyme-like function of prebiotically plausible heterogeneous polymers. Finally, through a top down approach we study the evolution of the modern cellular structure.

### **B6. What was the nature of the first genetic systems employed in the "progenote"?**

We seek to go beyond the goal of understanding the last common ancestor of archaea, bacteria, and eukarya (LAABE; commonly presented as the LUCA). Starting from simple pre-biotic compounds which formed complex and functioning large molecules, life was born as a community. What was the gene set of the first community like? How did these genes "flow" between community members? What are the factors that enabled sustainable and evolvable ecosystems to be built? In addition, where was the initial environment located that was able to utilize 20 kinds of amino acid and genetic codes? How did it become a life system? We approach those fundamental problems experimentally.

We lead the field of OOL (Origins of Life) by re-framing the question of what life's emergence means: it is not one stage but many stages, which could have involved many planetary locations and processes. We introduce the premise that the creation of biochemistry did not only take place in the evolutionary era of cells, but began in geochemical processes that produced and partially selected complex organics, and continued in later cellular eras. Similarly, cellularization included stages of producing components and then combining them into functioning systems.

### **C) Evolution of the Earth-Life system**

After the emergence of life on Earth, the biosphere and the crust/atmosphere/ocean system co-evolved in composition and complexity. We aim to understand and ultimately to reconstruct stages in this coevolution, through a joint study of the geological record and the comparative analysis of molecular diversity in the biosphere today. Our investigations here are directed at three aspects of long-term evolutionary change: (1) major transitions in the bioenergetic systems that organisms achieve to enable biochemistry and physiology on a changing planet, (2) what molecular comparative analysis and synthetic biology can tell us about long-term changes in gene architecture and enzyme function across time, and how to reconstruct experimental models of ancestral states, and (3) how long-term secular changes from thermal evolution of the Earth combined with Earth-life co-evolution to change the surface environment for life.

#### **C7. What were the major transitions in bioenergetic systems, what drove them, and how did they affect the spread of life?**

The evolution of life from the Hadean eon to the present has in many ways been an evolution in methods that couple energy-releasing physical processes to energy-requiring biochemical processes. The two primary forms of life's energy metabolisms have been chemotrophy — utilization of the disequilibrium between the bulk Earth and the atmosphere/ocean system — and phototrophy — coupling of chemical transformations to the absorption of light and emission of heat. Life during the Archean evolved several qualitative innovations in chemotrophy that allowed it to colonize ever more diverse and extreme environments, and that led to increasing ecological complexity. Sometime in the Archean, life also evolved the capacity to harness sunlight to drive biosynthetic chemistry and physiology. After many innovations in phototrophy, the latest — oxygenic photosynthesis — ended the Archean EON and began the Proterozoic, so completely did it change the surface geological environment. Changes in bioenergetic systems may have been partly driven by changes due to thermal evolution of the solid Earth (considered in C9). They unquestionably fed back to change most aspects of the surface environment, from mineralogy to Carbon chemistry, and altered the nature of subsequent evolution. ELSI will seek to understand both the historical sequence and the geological and evolutionary constraints and causes of innovation in bioenergetic systems throughout the Archean, and how these enabled the specialization and spread of life on Earth.

#### **C8. How were ancient enzymes and genomes different from modern ones, and can we reconstruct models of ancestral phenotypes?**

As biochemistry and bioenergetics have co-evolved with changes in geochemistry (C7), the functions of the two key informational molecule classes — polypeptides and polynucleotides — have also changed in form and complexity. Additionally, their organization in both genomes and ecosystems has done the same. Information about these changes is recorded in the diversity of molecular sequences among living organisms today. It can be extracted by established comparative methods of molecular biology, and are augmented by new techniques in single-cell genomics and laboratory experimentation aimed at understanding fundamental mechanisms of molecular interaction that have governed evolution at all historical periods. At ELSI we combine comparative and functional analysis with synthetic biology tools, not only to infer ancestral states but also to construct functioning models of ancestral phenotypes in the laboratory. Our efforts will focus on i) the evolution of pathways for autotrophic carbon fixation, which is a fundamental function that has governed evolution at all stages in life's history and ii) sulfur metabolisms and the enzymes which facilitate them. These catalyst classes provide links between the origin of the first cells, contemporary energy metabolism, and also Earth evolution.

#### **C9. How did the thermal evolution of the solid Earth change the ecosystem?**

We will explore how the long-term cooling of the solid Earth influenced the co-evolution of life, atmosphere and ocean. We will elucidate the changes in the chemically-stratified structure of the Earth's interior over time based on convection simulations with parameters defined by our high pressure experiments (A3), and we will evaluate the intensity of the volcanic activities and growth rate of continents. Using the physical properties of the core determined by A3, we will perform numerical simulations of the convection in the core and its change through time. We will estimate the timing of the birth of the inner core, which probably changed the geomagnetic intensity. In addition, using the geological samples, we will analyze paleogeomagnetic intensity through time, large-scale volcanic activity, continental growth, and we will thoroughly verify the simulation results. Taking the surface environmental changes brought by the solid earth evolution into account, we will re-evaluate the causes of the two evolutionary events: the emergence of eukaryotes and the emergence of metazoans.

## **D) Bioplanet in the universe**

A common emphasis in all of sections A—C is to understand the particular history of life on Earth as a realization of general principles of life that determine how and where it arises among the possible planetary conditions and histories. The goal of a universal planetology and a universal biology is to make generalizations and apply these to the characterization of planets throughout the universe in their capacity to generate or host life, to guide searches for life outside the Earth, and to understand what the search for the Origin of Life teaches us more generally about the nature of life as a planetary property.

### **D10. How unique is our planet?**

Through the study of Earth, obtained from A1 to C9, and by comparing Earth with the other terrestrial planets (in our solar system and possibly beyond), we will clarify both universal and unique aspects of our home planet. The next step is to attempt to generalize these aspects of Earth and construct a set of conditions that leads to “Bio-Planetology”. We base ‘Bio-Planetology’ on “Comparative Planetology”, which is the study of the complete set of extrasolar planets and understanding the underlying processes that generate the distribution of outcomes. With Bio-Planetology we aim to predict the presence or absence of life on other planets and what planets could be inhabited.

### **D11. How should we search for extraterrestrial life?**

We will work closely with those in the fields of space missions and astronomical observations, in order to apply the research results of the above points A to C for the detection of life on other planets, satellites and similar objects. Within the next 10 years, spectroscopic observations will start to yield information about the atmospheres of extra-solar Earth-like planets in the habitable zones, which may have oceans on their surface. Before that, we will establish criteria for life-harboring planets using the results of our explorations on the early Earth and its subsequent evolution. We will also actively participate in science discussions of an on-going space mission (Hayabusa-2) and lead science plan of future mission (MMX).

### **D12. What principles lead to life in a planetary context?**

To understand the scientific meaning of the origin of life, and the role of the biosphere as part of a planetary system, requires much more than a scenario for the origin of biomolecules or cells. This would be true even if we knew which scenario is the historically correct one: a history of empirical events does not distinguish which aspects of life are accidental and which are essential; it does not explain whether our biosphere is robust and if so, why; and it does not identify the key abstract properties that make living systems different in essential ways from nonliving ones. In practice, the search for scenarios for the emergence of life is so difficult that without a strong theoretical framework there is reduced likelihood that our proposed hypotheses will be valid. Therefore, guided by a deep understanding of the empirical and model-based analyses from A1 to C9, and drawing on theories of organization across physics, computer science, and the life sciences, we will work to define the abstract properties essential to the origin of life, and seek to quantitatively demonstrate conditions for their emergence in a planetary system.

## **[Social Impact]**

The ultimate goal of this study is to go back to the origin of science, and ask ourselves “why are we here?” There is no question that the results of our research activities will revolutionize our views of Earth and life, as state-of-the-art scientific achievements and the most advanced attainments of intellectual and cultural activity of human beings. Our research will stimulate young people who will carry the future of the scientific nation of Japan by reminding them of the intellectual desire and curiosity that is the original instinct of human beings, through which they distinguished themselves from other creatures.

Each research plan is conducted with clear scientific objectives while developing new advanced techniques. As a result, there are countless effects on the society in the short term. For example, development of techniques for ultra-high-pressure and ultra-high-temperature experiments; development of high speed large-scale computer systems; design and development of organic molecules on the basis of chemical evolution experiments; finding previously unrecognized factors controlling global environmental change; innovation of advanced techniques of environmental measurements, analysis and decoding; discovery and a wide spectrum of application of novel and unique extremophilic microorganisms; large-scale acquisition of microbial genetic information and resources; developing, analyzing and mining enormous quantities of genomic data; making progress in space exploration technology driven by the intellectual desire of human beings, and so on. However, these short-term impacts are only by-products of this program.

## **[Research plan]**

We will try to answer the above 12 questions from A1 to D12 through interdisciplinary investigations. Each research plan is described in detail below.

## A1. How was the Earth formed?

We aim at theoretical understanding of Earth formation from formation and evolution of protoplanetary disks through late impacts to the Earth by leftover planetesimals. We utilize first principle simulations and combine their results to build a general planet formation model by calibration with astronomical observational data of extra-solar planets and geo/cosmochemical data of our solar system.

The important physical processes that were not considered in the classical model are protoplanetary disk evolution, accretion of disk gas, dust grain growth to pebbles in turbulent disk, pebble formation/migration, pebble accretion by planets, planetary orbital migration due to planet-disk interactions, tidal orbital evolution, and orbital instability. Observations of protoplanetary disks developed since the 1990's after establishment of the classical model and recent observations by ALMA radio telescope provide amazing information of the disks. Grain growth in turbulent disks is recently understood by high-performance computer simulations, and pebble accretion has been proposed that would be equally important to the classical idea of planetesimal accretion. The importance of orbital evolution due to planet-disk interactions, star-planet tidal interactions, and instability has been highlighted by discovery of diverse extra-solar planets. We build a general planet formation model by incorporating these new processes to discuss the Earth formation process on the basis of the general model.

Recent development of computer simulations enables us to simulate impact history to the Earth after its formation. The giant impact that formed the Moon is essentially important for mixing of Earth's interior and evolution of initial atmosphere and ocean. The late impacts by leftover planetesimals are essentially important to infer surface environments of early Earth where life may have emerged. The theoretical results have become detailed enough to be compared with geo-chemical data. The computer simulations are now revealing formation history of Mars and asteroid belt as well, which can be compared with cosmochemical data of meteorites from there. We combine high-performance computer simulations with the geo/comso-chemical data to reveal the first 500 M year history of the Earth from dynamical point of view.

The temperature of the disk regions where building blocks of the Earth were formed, was not low enough for volatile elements such as H<sub>2</sub>O ice and organic molecules to condense there. In a protoplanetary disk, H<sub>2</sub>O ice dust can be condensed from the disk gas only in regions beyond 3AU with temperature below 160-170K. Even if planets are located in habitable zones, they may not be able to harbor life without H<sub>2</sub>O and organic molecules. We explore how H<sub>2</sub>O and organic molecules are delivered to planets in habitable zones including our Earth, using the new planet formation model and high-performance computer simulations. One idea to deliver water to the Earth is accidental impacts of asteroids or comets formed beyond 3AU. As scattering phenomena are chaotic, simulations show that delivered water is distributed broadly from zero to tens of wt% of Earth's mass. The coexistence of ocean and land could also be a condition for a planet for life to emerge (the Earth's ocean mass is 1/10000 wt% of the Earth's mass). If this mechanism is responsible for the water delivery, creation of life is determined by pure coincidence. We will re-examine this model, on the basis of the rebuilt planet formation model. We will also investigate other possibilities such as formation of H<sub>2</sub>O by interaction between a primitive hydrogen atmosphere and a magma ocean (Genda and Ikoma, 2008) and a new pebble accretion model for planet formation (Sato, Okuzumi, Ida, 2016).

Internal ocean of an icy satellite (Europa or Enceladus) is one of possible sites where life exists. Icy satellites of gas giant planets are believed to form in circum-planetary disks in a similar way to planet formation in circumstellar protoplanetary disks. The standard model of icy satellite formation has not been established at all. We also build the satellite formation model by applying the new planet formation model.

Experimental studies are also important. It is important to identify the chemical composition of the lower mantle, which accounts for 60% of the volume of the earth and the light element content in the metallic core, in order to elucidate the original composition of the Earth. Our ultra-high-pressure experiments with geochemical/geophysical information can constrain the original concentration of volatile elements such as O, S, and Si in the metallic core, resulting in great progress in the elucidation of the Earth's building blocks. How much water can be included in the mantle and the core is also important to constrain the water delivery process. The total amount of ocean is only 0.02 wt.%. It is likely that the mantle and the core can include water much larger than the ocean mass. These establish important boundary conditions for the simulation of the formation process of the early solar system and elucidate how the Earth was formed, and its uniqueness and universality in the planet formation process.

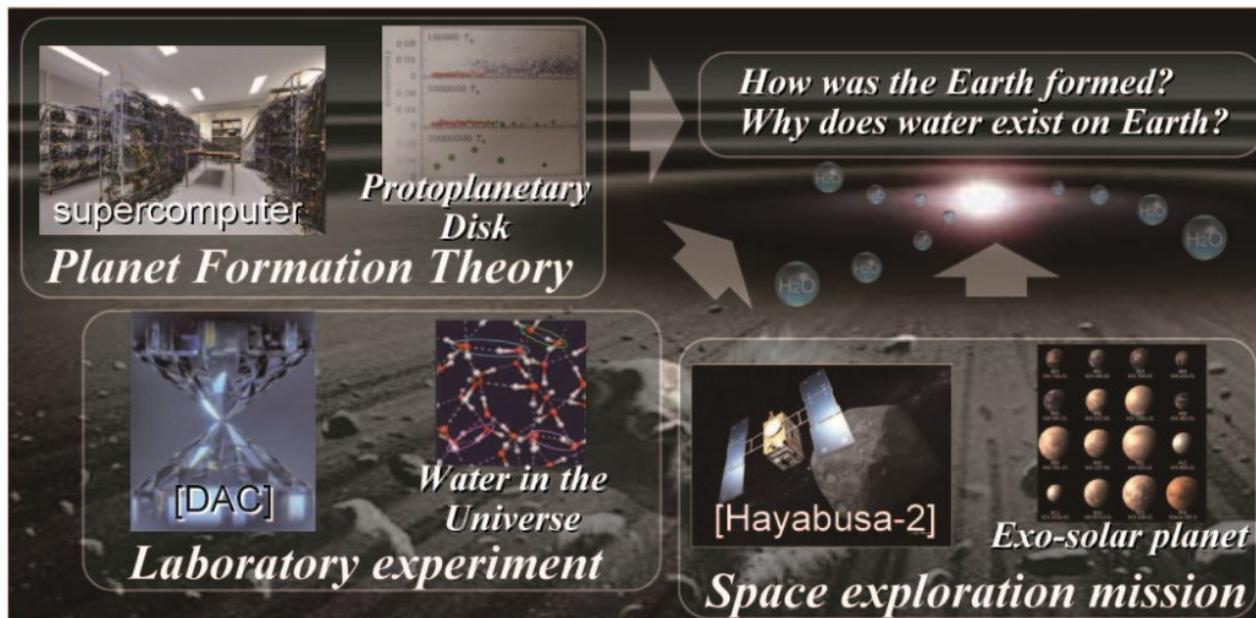


Figure 2. The formation of the Earth in the solar system will be examined by a combination of computer simulations of planet formation, with the aid of laboratory experiments and information about extraterrestrial bodies (related to question **A1**).

**A2. How did the “magma ocean” phase connect early formation/differentiation to conditions when life emerged, including the essential element of water?**

At ELSI we have assembled a diverse team of leaders in magma ocean studies, ranging in background from planetary formation theorists, atmosphere modelers, geodynamicists, mineral physicists, and geochemists. As a collaborative fusion effort we are now organizing activities around particular aspects of the problem that require very diverse expertise and assembling teams to solve some of the greatest questions in Earth science. ELSI PIs Hirose, Ida, Hernlund, and Helffrich are anchoring ELSI efforts to create this bridge between planet formation modeling and early planetary evolution.

**Informing evolution models with high-pressure experiments:** Our ELSI team has both modelers and high-pressure experimentalists who already have experience working together to bridge results from their disciplines. The important connection between them is that models can only make concrete predictions if they are constrained by reliable experimental data regarding physical and chemical properties. Sometimes models can use existing experimental data, but often in the course of investigation it is necessary to find new constraints and so a productive and synergistic feedback loop can be established between the modeling and experimental teams. Magma oceans are also an excellent opportunity to form a bridge between planet formation modeling and geodynamical modeling, and understand the physics of the planet assembly and subsequent evolution in an integrated manner.

**The primordial ocean and atmosphere:** Magma oceans simultaneously equilibrate with metals that form the core and with the proto-atmosphere that will partly condense to form the first water ocean (B4). Magma can readily absorb high amounts of water, and therefore acts as a conduit for early volatile distribution between the deep Earth and surface environment. Furthermore, the presence of volatiles exerts an important feedback upon the dynamical evolution of magma oceans. The outcome is sensitive to the timing and amount of volatiles delivered to Earth. We will combine our models of volatile delivery to the proto-Earth with magma ocean evolution scenarios in order to map out the range of potential behavior. The results of these models will inform targets for high-pressure experiments that can be used to test hypotheses and narrow the range of uncertainty.

**The first crust:** The solidification of the magma ocean following the late stages of accretion produced the very first solid surface of the planet. The “first crust” is an important target because the chemical environment it establishes will govern the kinds of organic chemical reactions that can take place, by regulating the supply of bio-elements and also providing energy sources for early metabolism (B4, B5). We may also find strong evidence that the first crust was not conducive to life, and therefore had to be replaced or modified by later geological processes in order to allow for the origin of life on Earth. We will

combine fluid dynamical models of magma freezing processes with petrological data that govern the fractionation of elements during crystallization and allow us to predict the composition of the first crust.

***Understanding the Diversity of Planets:*** Magma oceans are planetary forges, and as such they are responsible for producing planetary diversity in the solar system and elsewhere in the universe. A better understanding of the earliest stages is fundamentally important for making predictions regarding the state and habitability of exoplanets (D10, D11) based on primary astronomical data such as the distribution of planet sizes and epicentral distance. Using forward models constrained by high-pressure experiments, we aim to discover how planets of different kinds can be formed as an outcome of distinct evolutionary histories during the magma ocean phase, and make predictions regarding their evolved states. This positions fundamental research conducted at ELSI firmly in the center of upcoming exoplanetary observation missions, because it will address the connection between planet formation, evolution, and current state (only the latter can be directly observed). This timely contribution is an investment that will ensure ELSI's relevance and maintain its high profile into coming decades.

### **A3. How has the Earth's structure, composition, and dynamics evolved through time?**

***Lower mantle:*** First, we need to clarify the structure and chemical composition of the lower mantle, which composes 60% of Earth in mass. ELSI members have already proposed the existence of silica-enriched viscous domains (bridgmanite-enriched ancient mantle structures, BEAMS) in the lower mantle, which is different in composition from the upper mantle material. In the next five years, we will need to find firm evidence for its presence. Moreover, we will explore how such compositionally-distinct domains were formed based on high-pressure experiments and computational simulations. These will tell us 1) how a magma ocean solidified, and 2) the chemical compositions of Earth building blocks.

***Core composition:*** The chemical composition of the core is one of the most important problems in the solid Earth science. Our high-pressure experiments and computational simulations will clarify the sound velocity and density of liquid Fe-alloys, differentiation of light elements at the inner core boundary, and the dissolution of light elements from the molten mantle into the core at the giant impact events on the early Earth, all of which provide important constraints on the identification of core light elements.

The determination of chemical compositions of the lower mantle and core will elucidate the bulk Earth composition. Then, comparing the result with cosmic abundances of refractory elements, we can examine consistency with the theoretically-derived Earth-formation scenarios obtained in A1 above.

***Magma ocean and proto-crust:*** We also examine the primordial layered structure inside the Earth, from the core to the proto-crust. We will reproduce experimentally the solidification of the magma ocean, which most likely extended to the whole mantle at the time of the Moon-forming giant impact event. While it has been believed that its solidification occurred from the bottom, recent experimental and theoretical studies suggest that magma is denser than surrounding solid and thus solidification started at the middle of the mantle, eventually spreading upward and downward, which changes the whole view of the solidification process.

The chemical composition of the Earth's proto-crust forming from the final residual melt after extensive crystallization of the magma ocean may have been significantly enriched in incompatible elements including phosphorus, the essential element for life. Indeed, the unusual type of rock called KREEP (K, REE, P-enriched) is found on the Moon's crust, but it can be different from the Earth's.

***Core evolution and geomagnetic field:*** Working from an improved understanding of its composition, we study the thermal and dynamical evolution of the Earth's core. Based on interdisciplinary collaboration between ELSI members, we have recently revealed that the Earth's core has changed its composition to a large extent by crystallizing SiO<sub>2</sub> oxide. Despite our discovery of high thermal conductivity of the core, convection has been driven by chemical buoyancy associated with SiO<sub>2</sub> crystallization, which may have formed Earth's geomagnetic field since its early history.

At the same time, by using vast amounts of Precambrian rock samples collected by our geology team, changes in paleomagnetic intensity will be examined. We will apply new techniques developed mainly by the PI, Kirschvink to improve the database of paleogeomagnetic intensity for Precambrian times, and thereby test the predicted changes. Numerous intrusive complexes from large igneous provinces are being discovered and dated accurately with U/Pb techniques, and simple shallow drilling operations could provide pristine samples amenable to the modified Thellier/Thellier techniques needed for robust paleointensity determinations. Magnetic microscopy using Superconducting Quantum Interference Device (SQUID) technology may even allow these techniques to be used on detrital grains of Hadean age. These studies are link with the theme C8.

***Surface conditions and influence of the galactic environment:*** Conditions on the surface of the solid Earth are governed by the interface with the atmosphere, a system locally protected by the

geomagnetic field, but at the same time influenced by dynamics on scales as large as the galactic environment. It is known that cosmic forcing can change the surface environment of the Earth at small scales such as local meteorological changes (due to cosmic ray influence on cloud formation), but has also been proposed that such changes could be large enough to account for global freezing events (Kataoka, 2013, 2014; Nimura 2016), with important consequences for long-term evolution (Ebisuzaki, 2015). The influence of galaxy structure on atmospheric forcing is expected to come through the three major channels of (1) Large changes in star-formation rates, (2) Collisions between molecular clouds and the solar system, and (3) Supernova explosions in the vicinity of the solar system. Recent advances in simulation technologies led by the ELSI Fellow Makino and his team have enabled us to theoretically analyze the origin and evolution of our Milky Way Galaxy, leading to a view significantly different from common belief (Fujii, 2011; Baba, 2012, 2015, 2016). Whereas it was formerly assumed that the solar system followed a circle in the galaxy through roughly static spiral arms, the new work suggests both non-circular motion of the solar system and non-stationary maintenance of arms, with implications for star-forming rates and locations, and solar system interactions with resulting molecular clouds. These calculations may suggest links between a 150-million-years cycle of changes in Earth's climate and in the position of the solar system in our galaxy.

ELSI is fully equipped to investigate the solidification of the magma ocean and chemically-stratified structure of the mantle, as well as to determine the primordial crust composition. Studies on core and lower mantle described above are primarily based on property measurements and calculations of iron alloys and silicate minerals, employing high pressure and temperature ( $P$ - $T$ ) experiments and computational simulations. At this point, the Hirose team is the only group in the world which can simultaneously create extreme high  $P$ - $T$  conditions that exceed that of the center of the Earth (364 GPa, ~6000 K) by static experiments using the diamond-anvil cell (Tateno, Hirose et al., 2010, Science). Combining such leading-edge technology and synchrotron radiation X-rays, the group has achieved several outstanding results. These include the discovery of post-perovskite, a major mineral in the lowest mantle (Murakami, Hirose et al., 2004, Science), determination of the crystal structure of iron in the inner core, the discovery of a phase transition of FeO under outer-core pressure (Ozawa, Hirose et al., 2011, Science), and the discovery of the cubic structural phase of SiO<sub>2</sub> (Kuwayama, Hirose et al., 2005, Science). Furthermore, we have developed a new methodology for measuring properties such as the electrical and thermal conductivity (Ohta et al., 2008, Science; 2016, Nature), seismic velocity (Murakami et al., 2012, Nature), and element partitioning (Nomura et al., 2011, Nature; Hirose et al., Nature, in press) under high pressure, which resulted in making major breakthroughs. Also, pioneering research has been conducted on mantle materials by Irifune's team based on precise measurements in a multi-anvil apparatus (Irifune, 1994, Nature; Irifune et al., 1998; 2010, Science; Irifune et al., 2008, Nature; Irifune and Isshiki, 1998, Nature). More recently, they succeeded in making the first measurements of elastic wave velocity under lower mantle  $P$ - $T$  conditions. Meanwhile, as reported in Irifune et al. (2003, Nature), the team started applying the world's hardest nano-polycrystalline diamond for the multi-anvil apparatus. This technology is expected to enable precise experiments under the entire range of mantle conditions.

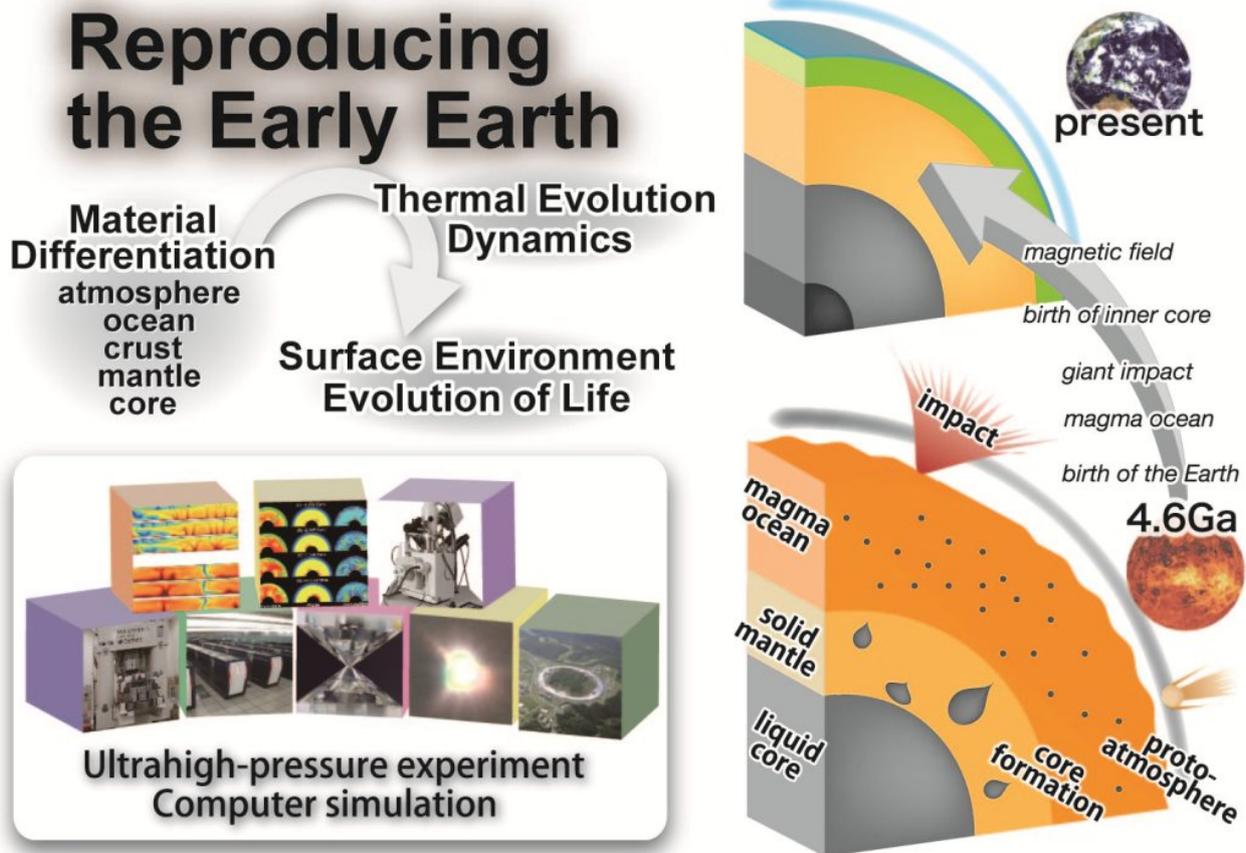


Figure 3. Chemical differentiation within the Earth from core to atmosphere will be reproduced by high-pressure/high-temperature experiments. Subsequent chemical and thermal evolutions inside the Earth will be also examined (related to question **A3**).

#### **B4. What was the state of the ocean and the atmosphere when life emerged?**

By extending the high-temperature experiments and theoretical computations of A1-3, we will make forward estimations of the composition of the atmosphere and oceans. To verify our theoretical predictions on the basis of geological evidence, we will analyze the early geological record dating back to 4 billion years ago.

**Theoretical and Experimental Approach:** Our objective is to specify the physico-chemical environment of the primordial Earth on which life emerged. According to the conventional theoretical model, the Earth's primordial atmosphere formed from volatiles (secondary atmosphere) produced by the degassing of planetesimals, the building blocks of the Earth. It is generally believed that the degassed volatiles consisted primarily of H<sub>2</sub>O vapor, CO<sub>2</sub> and N<sub>2</sub>. As the Earth's surface cooled, H<sub>2</sub>O turned to liquid (i.e. ocean), while a CO<sub>2</sub>-rich primordial atmosphere remained. Under such a CO<sub>2</sub>-rich (i.e. oxidizing) atmosphere, however, it is extremely difficult to follow pre-biotic synthesis of organic matters that are necessary for the emergence of life. On the other hand, recent research results rather suggest a more reducing primary atmosphere, possibly rich in H<sub>2</sub>, CH<sub>4</sub>, and CO based on theoretical calculation and geological evidence. It is also important to study resetting the atmospheric composition by reactions with meteorites that fell after the Magma Ocean. Our research at G-COE has suggested the possibility that the moon-forming impact ejected fragments that returned to Earth during 100 million years after the impact. These re-entering fragments may be large enough (10 to 100 times larger than impact from the Late Heavy Bombardment event) to have converted a substantial amount of primordial ocean into H<sub>2</sub> (Sasaki et al., 2012, in our team). Because these early atmospheric conditions also define the origins of H<sub>2</sub>O on Earth, they are extremely important for understanding the origins of seawater and its total volume as discussed in A1. For re-evaluating these new scenarios, we will first perform numerical simulations by extending the planet formation theories developed in A1. In particular, the H<sub>2</sub>O content of planetesimals and their accumulation process after solidification of the magma ocean are important aspects on which

we will focus in our simulations. Furthermore, the mass of the early atmosphere and oceans is controlled by the cooling process of the magma ocean that we can constrain by using the high-pressure experiments of A2 and A3.

In addition, the composition of the atmosphere was modified by gases released from the mantle through volcanic activity. This process has been studied on the basis of research using today's subaerial volcanoes. The early Earth, however, was covered with oceans and had almost no land. Hence, input to the atmosphere and ocean system would come not from high-temperature volcanic gases, but from submarine hydrothermal gases resulting from reactions between rock and seawater. Hence, we will perform hydrothermal experiments on rock types from the Earth's earliest oceanic crust determined by A3 to systematically understand the volatile and elemental flux into the early atmosphere and oceans. The experimental setup has already been developed and utilized to study this issue by the group of the ELSI Fellow, Takai and PI Maruyama (e.g., Yoshizaki et al., 2010).

***Geological and Geochemical approach:*** Our theoretical predictions must be thoroughly verified on the basis of geological evidence. Unfortunately, the means for such verification for the Earth's environment during the Hadean (before 4.0 billion years ago) are extremely limited because there is no geological record except for tiny mineral grains in clastic rocks. In the past ten years, however, dramatic advances in research on the early ocean and atmosphere during the Archean (4.0 to 2.5 billion years ago) have been made by rapidly developing chemical and isotopic indicators recorded in sedimentary rocks that now provide useful boundary conditions to verify the Hadean environment. In particular, 1) over 10 years of geologic mapping of the PI, Maruyama's group has identified many fragments of the past oceanic crust in Archean cratons and their comprehensive metamorphic petrology, making it now possible to quantify the CO<sub>2</sub> concentrations in the Archean ocean (e.g., Nakamura et al., 2004; Shibuya et al., 2007; 2012, in our team). Moreover, 2) after the discovery of a sulfur isotope anomaly in Archean sedimentary rocks that proved extremely low oxygen levels of the Archean atmosphere (Farquhar et al., 2000), recent advances in research on the isotope fractionation of photochemistry makes it possible to quantify not only oxygen levels but also the concentration of green-house gases and volcanic flux into the atmosphere (Lyons, 2007; Danielache et al., 2008; Ueno et al., 2009, in our team).

In this context, we will reproduce the composition of the Archean oceans by using systematic chemical and isotopic analysis with thermodynamic computations on the rock samples. Tokyo Tech's Earth history archives already house numerous Archean oceanic crust samples. While we have already obtained fixed-point data based primarily on detailed field mapping in designated regions and metamorphic petrology, we will now significantly broaden our scope in order to describe temporal changes across the entire Archean. For decoding the Archean atmosphere, while much data has been collected on isotopic anomalies regarding their role as atmospheric proxies, the inherent potential of this research has not been fully realized because the basic mechanisms for producing the isotope anomaly are still inadequately understood. Hence we will conduct spectroscopic studies and reaction experiments with numerical simulations of photochemical reactions to understand the dependencies of UV wavelength, atmospheric composition, temperature and pressure on the isotopic effects in order to constrain the Archean atmosphere quantitatively. The PI, Yoshida and his group has determined photochemical isotope effects by a number of key reaction steps (e.g., Danielache et al., 2008; Ueno et al., 2009; Hattori et al., 2011; Enghoff et al., 2012) and will extend this research to produce testable models of the Archean atmosphere by using geologically preserved isotope anomalies.

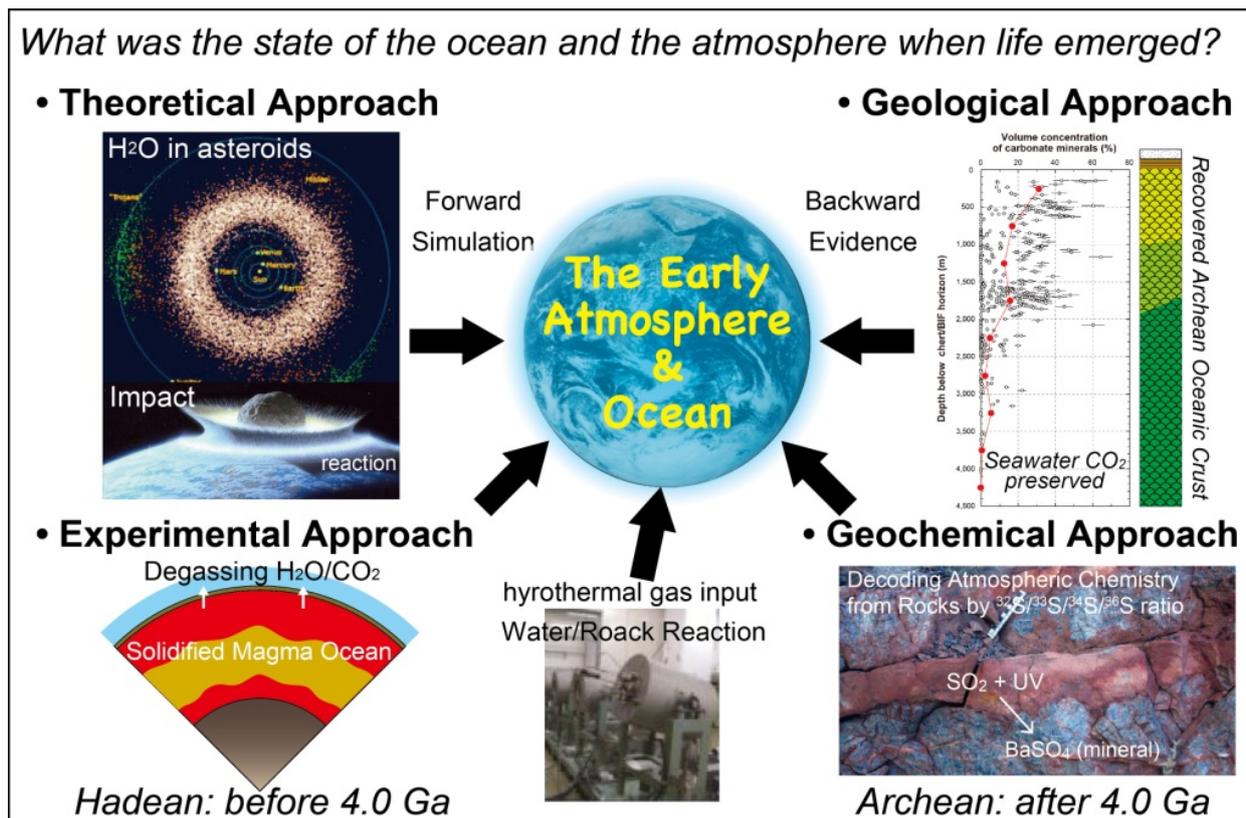


Figure 4. Chemistry of the early atmosphere and oceans will be determined by planet formation theory and tested by geological evidence (related to question **B4**).

**B5. How did the geological conditions of the early Earth influence the origin of life?**  
*How did the geological phenomena influence the prebiotic chemistry?*

Triggered by interdisciplinary studies that have promoted as JSPS KAKENHI Grant-in-Aid for Scientific Research on Innovative Areas “Hadean Bioscience,” which launched in 2013, the Institute PI Shinegori Maruyama et al. proposed the “natural nuclear geyser scenario” (Maruyama and Ebisuzaki, 2016), which presumes that the radioactive placer deposits could have formed the geyser system as water and radioactive minerals reacted in a fashion similar to that in modern nuclear reactors. Utilizing the  $\gamma$ -radiation facility at Tokyo Tech, the research team led by ELSI Fellow Masashi Aono and H. James Cleaves has initiated the radiolysis experiment designed to mimic the radiation-induced syntheses of organic compounds in the natural nuclear geyser and succeeded in converting water and acetonitrile to formamide (results to be submitted soon), which offers promising prospects for abiotic synthesis of building blocks of life (e.g., amino acids, nucleobases, and lipids). Inspired by the geyser concept, Aono and collaborators have developed a so-called “geyser reactor,” an intermittent experimental setup that repeats the wet-dry cycle in a confined flask, and demonstrated amino acid oligomerization by high-temperature heating without a catalyst (results to be submitted soon). Catalytic amino acid polymerization is investigated at ELSI as well, specifically polymerization on mineral surfaces. Amino acids undergoing polymerization in the presence of minerals, e.g. pyrite, are assumed to adsorb and condense only on specific surface sites. Quantitative measurements of amino acid adsorption on the pyrite surface using atomic force microscopy (Narangerel et al., 2016) are expected to elucidate the mechanism of prebiotically reasonable peptide formation. Further investigations into radioactivity-induced chemistry inspired by the natural nuclear geyser scenario and mineral surface driven polymerizations will become core areas of inquiry connecting early Earth and Life.

**Can “messy” prebiotic chemistry sustain life-like processes?**

Nuclear geyser reactor could have initiated and sustained prebiotic chemical networks capable of synthesizing biological building blocks and possibly sustaining life-like processes. Other notable examples of similar systems include Miller-Urey experiment (Miller, 1953), HCN (Moser et. al., 1968) and formaldehyde polymerization (Cody et. al., 2011). There is a commonality to most of these systems —

they are qualitatively messy. The systems produce large assortments of compounds through a wide variety of mechanisms. Biological systems are strikingly different; they are well-orchestrated enzyme-controlled networks. How did the transition from prebiotic messy chemistry to the organized biology resembling reaction network occur? In our goal to shed light on the issue we employ a number of approaches. An effort fronted by Nathaniel Virgo concentrates on artificial chemistry, the study of abstract artificial chemical reaction networks and their emergent dynamical properties. Virgo's prior work in collaboration with Takashi Ikegami of the University of Tokyo suggests that simple chemistries in the thermodynamically reversible regime can self-organize to form complex autocatalytic cycles, with the catalytic effects emerging from the network structure (Virgo et. al., 2016). Further inquiries will include in depth study of intermolecular interaction driven self-organization of complex reaction networks, both experimentally and *in silico*. Polymers formed by the messy chemistry might have played an important role in chemical evolution, e.g., as prebiotic enzyme mimics. In modern biology the control over complex metabolic networks is achieved through the use of enzymes. Enzymes are intricate biopolymeric complexes that catalyze biochemical reactions and shape metabolic pathways. Enzymes usually work with small molecule cofactors that actively participate in reaction mechanisms and complex, usually globular, polymeric structures capable of specific substrate binding, encapsulation and orientation. Moreover, the globular structures of enzymes possess cavities with modulated microenvironments, facilitating the progression of reaction(s). The globular structure is assured by long folded protein or RNA strands. Synthesis of such elaborate complexes has proven difficult under prebiotically plausible conditions. In our endeavors we consider the concept of protoenzyme, an enzyme-like structure that uses alternative simpler polymeric scaffolds derived from the "tarry" prebiotically plausible materials. Research efforts fronted by Mamajanov, ELSI PI, are based on *hyperbranched* polymers, macromolecules with a high degree of branching assuring their globular structure. The recent study (Mamajanov and Cody, submitted) has successfully shown the ability of unresolved mixtures of tertiary amine-bearing hyperbranched polyesters to form hydrophobic pockets as a reaction promoting medium for the Kemp elimination reaction. Further studies will involve hyperbranched polymer based metalloenzyme mimics.

### ***Did electrochemical processes triggered by the hydrothermal vents constrain the "messy chemistry"?***

Hydrothermal vents on the early Earth were likely to have been more active than they are now (Shibuya, Takai, et al., 2016). The geo-electrochemical potentials they provided could have served as a driving force for the CO<sub>2</sub> reduction followed by the formation of organic compounds essential for the origin and early evolution of life (Kitadai, et al., 2016). We have designed an array of experimental setups that can simulate electrochemically driven CO<sub>2</sub> reduction and help evaluate the reaction energetics and estimate the catalytic potential of the geothermal environment. While ELSI Fellow Takai and collaborators excel at discovering the diversity and properties of deep-sea hydrothermal vents, the research effort lead by Shawn McGlynn (ELSI PI), Norio Kitadai (ELSI Research Scientist) and Riyuhei Nakamura (newly appointed ELSI PI) are applying the newly discerned parameters to the prebiotic chemistry studies. The outcome of their studies will not only elucidate the chemistry relevant to transition between geochemistry to biochemistry at the early stages of chemical evolution (Aono et al., 2015), but will also provide relevant constraints for future JAXA and/or NASA space missions targeting the search of extraterrestrial life. Hydrothermal activities are believed to be present on the surfaces of certain planets and satellites found in the Solar System (Kurokawa et al., 2014).

### ***What is the role of compartmentalization in the emergence of life?***

Compartmentalization is yet another means to restrict the diversity of prebiotic chemistry as it would limit the diffusion of chemical towards and away from a given chemical system. Besides, compartmentalization in a form of cell is a necessary attribute of life as we know it. A program led by Yutetsu Kuruma sets an ambitious goal of elucidation of the formation and subsequent evolution of the cellular membrane, from the theories of the protocell to the cell of nascent biology to the contemporary cell. Lipid membrane vesicle is crucial as an outer envelope of cell. All necessary metabolisms, glycolysis, gene replication, gene expression, lipid synthesis, and energy production, must be set up within the vesicle. Especially, lipid synthesis is important process because it directly leads the self-reproduction of cell. According to Mercier and Kawai et al. (2013, Cell), only a continuous over-biosynthesis of lipid molecules is enough for cell division even without the cell wall and cell division machineries such as FtsZ ring formation. This style of division is called as L-form, and it is thought to have occurred in early stages in the emergence of cell. In order to verify this phenomenon by constructive approach, we try to reconstruct the metabolic system of lipid synthesis by combining responsible enzymes, substrates, and co-factors.

Fatty acid is a basic structure constructing phospholipids and synthesized by 8 kinds of Fab (fatty acid binding) enzyme, ACP (acyl carrier protein) and TesA. These enzymes elongate hydrocarbon chain from the resource of acetyl-CoA and malonyl-CoA. We have so far finished the purification of the enzymes and will try to drive fatty acid synthesis reaction inside a lipid vesicle of artificial cell. Detecting the morphological change of artificial cell where lipids are synthesized and supplied onto the membrane, we try to clarify the condition of cell division in very early stages of cellular life and how first cells evolved to the modern cell form.

The transition between geo- and biochemistry is a multifaceted question. A satisfactory answer requires a multidisciplinary research program merging the expertise of a number of branches of physical sciences, which is certainly descriptive of ELSI.

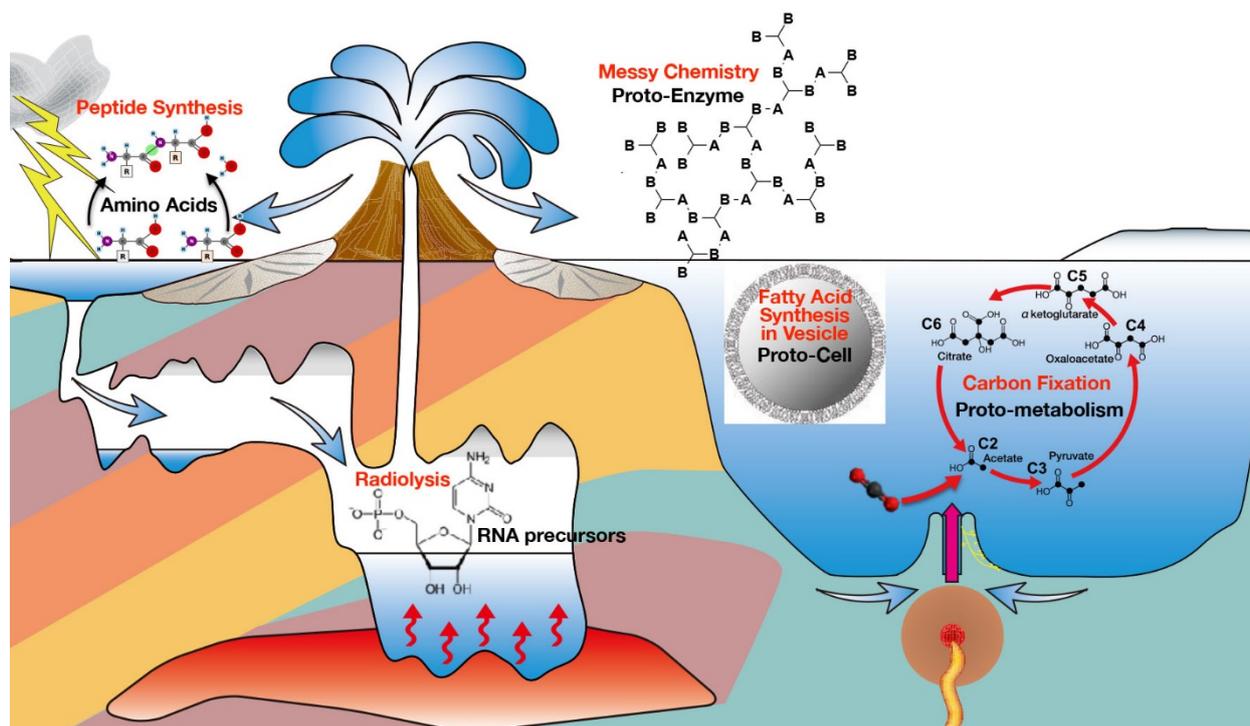


Figure 5. Schematic representation of the scope of the ELSI research into geologically driven chemical evolution. Formation of simple biological building blocks, polymers and larger functional supramolecular assemblies will be investigated (related to question B5).

### B6. What was the nature of the first genetic systems employed in the "progenote"?

To achieve a sustainable and stable existence without extinction, a robust life system was necessary, yet certainly many – perhaps even most – ancient lineages became extinct. Those that survived did so by chance and selection, resulting in cellular and ecological systems which could cope with environmental disruptions. While research on the robustness of cellular systems has progressed in the life sciences and ecological systems, very little has been done to consider community robustness in an era prior to the emergence of phylogenetically distinct lineages. This area of research will therefore aim to elucidate dynamics that produce ecosystems that are both sustainable and capable of evolving in the absence of a strict dependence on vertical inheritance; it is undertaken with the objective of tracing genomic diversification and ecosystem formation which led to the formation of life as we know it today.

#### *How did peptide: nucleic acid interactions proceed to the point of translation?*

An important aspect of early systems concerns i) the type of amino acids initially used for protein construction and ii) how did these amino acids become recognizable to oligonucleotides. In previous sections B4 and B5, we have dealt with the chemical environment of the early Earth, as well as the relationship of this environment to the formation and interactions between small molecules which may have been substrates for the first living systems. Here, we ask deeper questions as to how these molecules could have interacted in *self referencing* ways. Since polymers hold considerable potential to act in self

referencing ways, and since the LAABE used a two component polymeric system based on peptides and oligonucleotides, we will investigate polymer-polymer interactions through a high throughput and combinatorial approach. Already, we have purchased a robot to conduct a high number of experiments towards these ends, and researchers Fujishima, Virgo, and Aubert-Kato are currently perusing these goals.

### ***How were Lipid Membranes originally functionalized by the progenote?***

For cellular life, the existence of the membrane is essential, and many origin of life researchers have sought to interpret the emergence of cells as connected to an ability to form a membrane structure. What is often forgotten though is that for a contemporary cell, up to ~50% of the total protein content can be associated with the membrane. This is a reflection of the membrane itself; while being a barrier, it is also *a pathway* of transport, and the totality of ion, molecular, and electron transport processes mediated selectively within and across the cell membrane together make up a critical functional aspect of what it means to be a living cell. Given this knowledge, our experiments led by Kuruma probe the ability of lipid membranes to become functionalized by proteins in artificial membrane models (Kuruma et al., 2015). Because all cells contain membrane-bound proteins, this work paves an important experimental thread for all theories of life's origin based on the emergence of cells.

### ***What form of energy utilization was used by progenote community members?***

All life forms utilize energy to organize and propagate their cellular material, and contemporary microbiology has revealed myriad ways that energy in the environment can be harnessed to power cellular construction and replication. Furthermore, the type of energy used by progenote community members, in addition to the mechanism of use by these members, remains almost completely unconstrained by experiment. Indeed, too often, experiments meant to investigate early cellular physiology have been run *as they approach equilibrium*, disregarding the observation that life itself operates as an open system and feeds off of energy from the environment for equally as valid of reasons as life feeds off of material from the environment – life operates away from equilibrium.

So, what was the first energy source which powered the organization of living systems? First we can note that all known life survives by employing electron transfer reactions (redox chemistry) of a form where electron flow from a negative to positive redox potential and this is associated with doing some form of work. We will address the nature of the first utilized electron sources and sinks using knowledge from contemporary biochemistry and microbial physiology, where we will consider molecules such as H<sub>2</sub>, S, CO<sub>2</sub>, as possible early energy sources in the form of favorable redox couples. We will also research the possibility that early (and contemporary) life may be powered by geo-electric currents. Of course, this experimental line is greatly informed by ELSI investigations into the nature of the first atmospheres and oceans (B4), as well as the molecular assemblages made possible through two polymer type molecular interactions and feedbacks.

We will establish whether or not the first organisms were chemiosmotic, or relied on other mechanisms of energy conservation such as substrate level phosphorylation and even alternatives such as thioesterification. We seek to establish the expected energy budget and cellular yields associated with progenote communities on this or other planets, and compare these data to our ELSI generated expectations of the state of the early Earth.

### ***What is a pathogen before vertical descent?***

In a world where vertical passage of information is not critical to community function, the idea that one member can become a parasite of another becomes significantly blurred, since freedom from the bindings of information passage by vertical transmission corresponds to a state where the health of any daughter cell is not required for the retention of genetic information. This curious situation may have only been possible at the time of the progenote, but it may have been a defining feature of the progenote community. Therefore, we seek to test the nature of "selfish" genes, cells, and their interactions in cases where information transfer can happen easily and frequently by what is known today as horizontal gene transfer. We seek to define "extinction" based on the propensity of *sequence retention* in an ecosystem, and also to shed light on the nature of evolution without vertical descent.

### ***What is the ecological positioning of viruses at the time of the progenote?***

It has been suggested by Forterre that viruses may have been ancient components of oligonucleotide based cellular processes. From this point of view, the evolution of RNA is most appropriately interpreted in the context of *competing and complimenting* cells and viruses. A major limitation on all evolutionary

interpretations involving viruses though, is that despite the fact that their abundance in the modern ecosystem outnumbers the cellular organisms in the order of magnitude, they remain vastly under sampled in comparison to cellular life. Simply, there are too few examples of known viruses from the natural environment, and from the ones which are known, we can be sure that very big surprises await in continued exploration of viral diversity. Because of this lack of knowledge, ELSI is pursuing a dedicated line of research aimed at advancing our knowledge of viruses and their interactions with host organisms. Preliminary data by our research group led by researcher Mochizuki suggests the possibility of alternative nucleobase utilization, and also novel viruses in various geothermal environments are being explored, including the Hakuba Happo onsen environment. The weak point of the RNA world theory is the chemical instability of RNA polymers, especially in thermal conditions. All modern organisms use more stable DNA as their genetic material, except for RNA viruses. As no RNA virus has been found from any thermophilic environment, the possibility of thermophilic RNA virus is currently being investigated.

***Microbial Ecology from the Perspective of the Individual:***

In considering the progenote, where vertical inheritance takes place to a lesser extent than to contemporary biology where vertical inheritance dominates, the evolutionary concept of the individual becomes blurred. If the progenote was comprised of cells, and if these cells horizontally exchanged DNA rather than vertically replicated it, what would be the metabolic relationships that could be expected to be in existence between community members? To begin addressing this question, we have begun to use analytical techniques which allow the visualization and discrimination of cellular activities within whole communities at the level of the individual. Already, PI McGlynn has conducted analyses over 5,000 individual and phylogenetically identified cells within a complex sedimentary matrix (McGlynn et al., Nature, 2015), and these techniques have subsequently revealed unprecedented variability within what were previously thought to be homogeneous populations (Kopf, McGlynn et al., 2015) and a novel mechanism of cellular interactions by direct interspecies electron transfer (Scheller, McGlynn, et al., Science, 2016). Now, we are using these same cutting edge techniques to better inform our understandings of cellular community interactions as they exist today. This data is the first of its kind and supplies a foundation from which to consider and hypothesize about the types of cellular interactions which were occurring at the stage of the progenote.

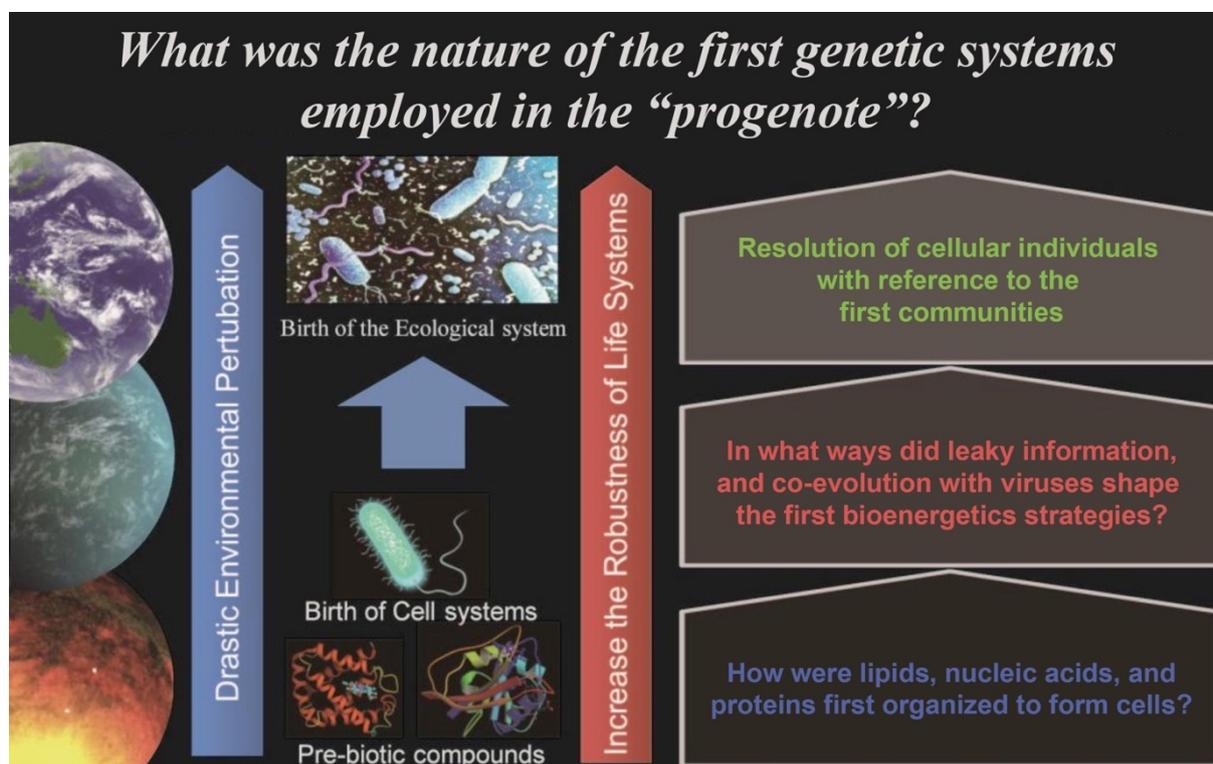


Figure 6. In-between a period of geochemically mediated (pre)biological transformations and the last common ancestor of archaea, bacteria, and eukarya, was a period known as the progenote (Woese, 1977); ELSI has become a forefront research center for investigating the progenote experimentally (related to question **B6**).

## **C7. What were the major transitions in bioenergetic systems, what drove them, and how did they affect the spread of life?**

Our research methods will be to combine wide-ranging molecular systematics and microbiology of the major carbon and energy metabolic pathways with high-resolution decoding of geological records to unravel the major evolutionary transitions in chemotrophy, and the innovations that led from chemotrophy to phototrophy, in the context of concurrent changes in the atmosphere/ocean system. We will address the following questions: What were the biological and environmental drivers of diversification and optimization of autotrophic carbon fixation pathways over time? Did early innovations in bioenergetics for Carbon-fixation pathways depend directly on geological processes such as the generation of electrochemical potentials? How complex are the changes in bioenergetic systems required to enable major reversals in biochemical pathways, which have occurred independently several times, and how is this complexity attained by organisms? These questions are major goals in the work of PI McGlynn and PI Nakamura. In what background of geology and biochemistry did the innovations of oxygenic photosynthesis arise? When and how did the atmosphere first become oxidized? Was the birth of eukaryotes caused by the rise of oxygen, and were Snowball Earth events crucial drivers of this transition? Placing geological and geochemical constraints on this transition is a major goal of PI Kirschvink and his group.

### ***Bioenergetic systems for autotrophic carbon fixation, and possible connections to geological electrochemistry***

One of the oldest Carbon fixation pathways is the pathway for direct reduction of one-Carbon units on cofactors, known as the Wood-Ljungdahl pathway. It is present in methanogens which branch deeply in tree of domain Archaea, and in acetogens deeply within the domain Bacteria, and has been suggested to be the first Carbon-fixation pathway. However, the bioenergetic systems used in these two branches are starkly different in their architecture, and each is highly optimized for the low-energy environments in which these organisms live. ELSI will seek to understand why these pathways diverged, and what more primitive bioenergetic systems could have supported them, as a path to understanding the origins of Carbon fixation. In particular, could such pathways have operated with less energetic optimization than they have in modern organisms, or augmented by different geochemical energy sources?

A connection of particular interest is the recent discovery by newly-joined (from April 2017) ELSI PI Ryuhei Nakamura, ELSI Fellow Ken Takai, and Masahiro Yamamoto at JAMSTEC, that hydrothermal environments which are known to host acetogens and methanogens also support direct electrochemical potentials (ordinary Voltages) across the walls of hydrothermal chimneys that stand between deep alteration fluids and unaltered seawater. Many experiments in the Nakamura lab, and also those by ELSI Research Scientist Norio Kitadai, have shown that one-Carbon reduction resembling that in the Wood-Ljungdahl pathway can be driven directly by electrochemical potentials mimicking vent potentials. We will seek to understand whether such geochemical supports led to either independent evolution, or gradual change, of the bioenergetic systems used by acetogens and methanogens, as well as whether any modern organisms use direct electrochemical potentials as their obligate bioenergetic system for carbon fixation.

### ***The “great reversals” in biochemistry, and how they were achieved bioenergetically***

The Wood-Ljungdahl pathway of methanogenesis and acetogenesis is not only used for Carbon fixation from CO<sub>2</sub>: when it is reversed it serves as a foundation for many varieties of carbon intake from reduced-Carbon sources, such as Anaerobic Methane Oxidation (ANME). This relation is probably one of the oldest of the “great reversals” that have occurred in biochemistry and is a major interest of PI McGlynn, who intends to collaborate with ELSI Fellow Kamagata on this topic. Another is the reversal from reductive Citric Acid cycling as a Carbon fixation pathway to the modern oxidative Citric Acid cycle (or Krebs cycle). The coupling of bioenergetic systems to biochemistry is different in important ways between oxidative and reductive directions in both pathways, but the differences do not require many new molecules and mechanisms, leading to the observation that modest molecular innovation and genome restructuring can lead to extensive metabolic change.

On the other hand, there have been during evolution the introduction of truly new types of molecular chemistry and energy too, for example that dealing with O<sub>2</sub> and light, which seems to have resulted in massive genomic modification and evolution. In addition to studying “reversible” energy metabolisms such as those discussed above, we will also seek to understand the determinants and evolutionary history of high potential (oxidizing) metabolisms such as that which works with O<sub>2</sub>. Here, we seek to derive knowledge on how the variables of metabolism, evolution, and Earth interact to establish novel chemistries during the prolonged evolutionary time scales experienced on the planet, and also during the shorter

scales which were relevant at life's emergence."

### ***Causes and consequences of the rise of oxygen on Earth***

The rise of oxygenic photosynthesis occurred in a context that was already highly complex with mechanisms derived from chemotrophy. At least two photosystem reaction centers existed (preserved independently in anoxygenic green-sulfur and purple bacteria); the major steps in chlorophyll biosynthesis were in place; the key carbon fixing enzyme (RuBisCO) appears to have existed in the group-IV outgroup, and auxiliary proteins such as the Carbonic Anhydrase were serving other functions in ancient groups such as methanogens. From the biological perspective, we will investigate the question of the rise of oxygen through the lens of ancestral enzyme state reconstruction linked to isotope fractionation factor determination. This effort, led by A-PI Kacar (Harvard satellite) represents a highly novel linkage of protein bioinformatics and genome analysis to the tools and data of geochemistry; namely isotope fractionation. The wedding of these two disciplines can be expected to result in insights into the evolution of enzymes (in biological catalyst evolution what comes first, specificity or velocity?) and also for the interpretation of isotope enrichments or depletions in ancient sediments.

The transition from chemosynthesis to photosynthesis must be recorded in Archean geological records. Recent development of stable isotope geochemistry has enabled us to identify the activity of some anaerobic metabolisms (e.g., methanogenesis and sulfate reduction) from isotopic information of Precambrian rocks. PI Yoshida's group, Ohkouchi and Ueno in our team have developed novel isotopic techniques to trace specific metabolic activities from geological rock samples (e.g., Ueno et al., 2006; 2008; Ohkouchi et al., 2007). Additionally, we have obtained information about anaerobic photosynthesis and other key metabolisms of anaerobic organisms are predicated by specific biochemical reactions to produce reaction centers – work which is led by ELSI researcher Tsukatani. In the nitrogen cycle, for example, nitrogen fixation, has been traced from within geological records by Fellow Takai's group (Nishizawa, Takai, and others, 2014).

We have explored proxies of biological metabolism in an analogous environment to anoxic early Earth and also with incubation experiments during the first half of the project. And we will also apply new techniques currently under development to geologic samples of isotope systematics (e.g., H, C, N, O, S, Fe) at the same time or during the second half of the project year, and we have also expanded our study environments of interest to include anaerobic hot springs which contain high concentrations of reduced iron, which is relevant to considering pre-oxygenic iron metabolisms. Conventional obstacles to this type of research have been metasomatic overprints and contamination of exotic compounds into sedimentary rocks long after deposition. There have also been technical obstacles that have prevented us from obtaining information from carbonaceous macromolecules (kerogen) in sediments, which should not be affected by post-depositional petroleum migration. Developing a method to overcome these technical difficulties is key. We will establish a new reliable geochemical method of extraction that focuses on organic nitrogen, hydrogen, and sulfur, and we will strive to develop techniques that can test for their syngenetic origin within their host rock. Consequently, we will unravel the evolution from chemosynthesis to photosynthesis in the realm of microorganisms based on geological evidence (e.g. Johnson, Kirschvink et al., 2013). The goal in our work will be to understand which factors in the origin of photosynthesis were of geophysical origin, which were evolutionary bottlenecks, and to determine what subset of these questions can be answered from evidence preserved in the geological record. We will also consider isotopic and fossil evidence connecting the rise of oxygen to the detailed timing of eukaryogenesis and the origin of multicellular animals, in C9.

# Why does the Earth's atmosphere contain oxygen?

## 1) Systematic & Evolutionary Biochemistry

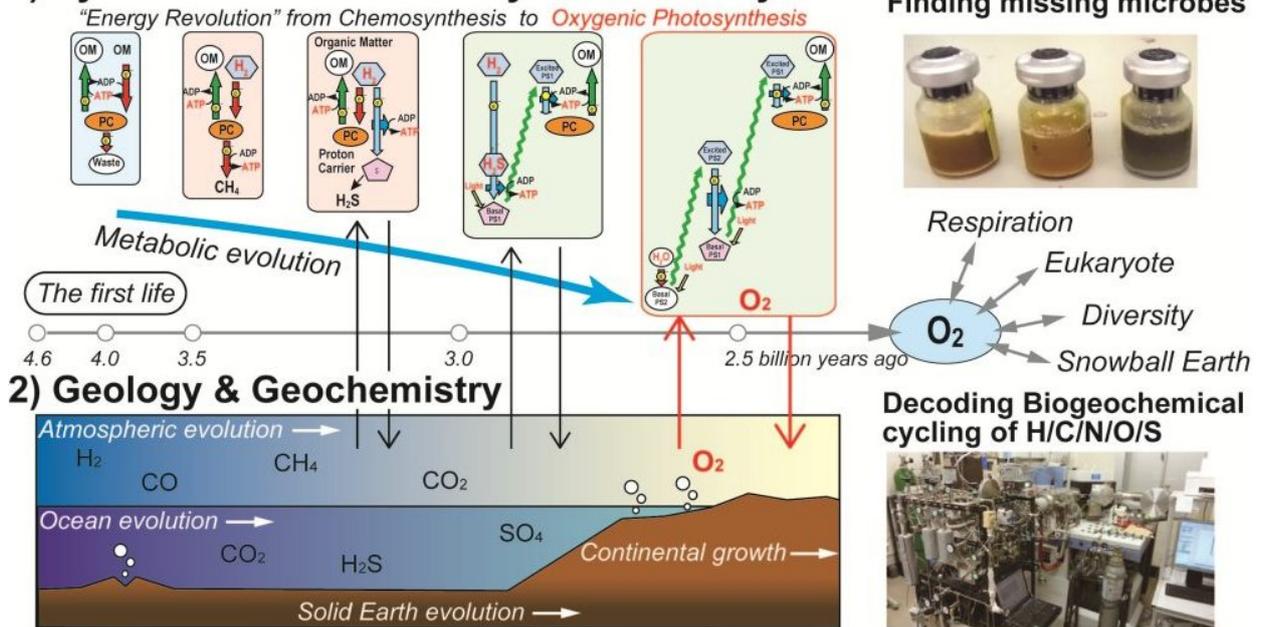


Figure 7. What drives major transitions in bioenergetic systems, and how do we accurately interpret these changes in the planetary perspective? We integrate biochemistry, isotopes, and geochemistry to uncover the relationships throughout time (related to question C7).

### C8. How were ancient enzymes and genomes different from modern ones, and can we reconstruct models of ancestral phenotypes?

ELSI research on molecular complexity and the reconstruction of ancestral phenotypes will concentrate in two areas. We will use comparative molecular systematics, microbial cultures, and empirical and computational protein biochemistry, to reconstruct protein sequences of a more primitive kind than any that exist on Earth today — a field known as “paleoenzymology” (Benner et al., 2007; Perez-Jimenez et al., 2011) — focusing on the enzymes in Carbon Fixation pathways. Then, we will join these comparative and functional studies with genomics and synthetic biology methods to assemble reconstructed ancient molecules into functioning systems or cells with truly primitive phenotypes, helping to create the next generation of evolutionary analysis, which we call “*molecular systems evolutionary biology*”. A particular area of emphasis will be to show how biochemical systems coevolved with bioenergetic systems and with changes in the geochemical environment, as developed in C7, as well as connecting evolution to the biological isotope record, which was ultimately derived from at the level of particular catalysts. In this way, we will link enzyme evolution, reaction mechanism, microbial physiology, and isotope geochemistry.

#### *Paleoenzymology of proteins in autotrophic carbon fixation pathways: Molecular systems evolutionary biology*

Molecular phylogenetics is an established method leading to hypotheses about the functions of ancient organisms and ecosystems. However, if quantitative methods are applied only to single sequences at a time (the current practice for most evolutionary reconstruction), the consistency of these hypotheses can be poor. The next step in evolutionary reasoning is to jointly reconstruct multiple interacting molecular histories, to deduce the evolutionary history of functioning systems by integrating knowledge from these histories. ELSI has three projects in process of this kind.

The first will reconstruct three ancestral-state proteins, which together are the ancestors of six of the eleven proteins in the reductive Citric Acid (rTCA) cycle of carbon fixation. This cycle, which is known to be one of the most ancient carbon-fixing pathways in the biosphere, was shown to possess three cases of enzyme homology suggesting that the catalysis performed by six specialized enzymes in modern organisms was once performed by three enzymes in the ancestor, each having two functions. This molecular fingerprint suggests an answer to a key puzzle of how organisms could have evolved complex functions

such as carbon fixation when they originally possessed only limited genomes and crude enzymes: the early enzymes were multi-functional precisely because they were crude. The work is a specialization of ELSI Research Scientist Masafumi Kameya, a former member of the laboratory that discovered these preserved homologies in the rTCA proteins. A second project, by Betul Kacar (ELSI A-PI in the Harvard satellite) aims to reconstruct sequences across the historic tree of the proteins RuBisCO and Carbonic Anhydrase which function in the Calvin-Benson cycle of carbon fixation uniquely associated with oxygenic photosynthesis. Our laboratories have all required capabilities to synthesize all reconstructed proteins, to test them for the hypothesized ancestral functions, and to determine using computational models which features determined their evolution from multi-functionality to selectivity. Both rTCA and Calvin-Benson cycle reconstructions are being performed in collaboration with ELSI PI Eric Smith and EON fellows Christopher Butch and Donato Giovannelli.

In a separate but related project, PI McGlynn/A-PI Kacar are pursuing reconstruction of the ancestral form of the CODH/ACS. In enzyme phylogenies, this enzyme cleanly splits the archaeal and bacterial domains and can therefore be interpreted as ancient. However, since all contemporary sequences are just that – relevant only today, the study of these proteins poses serious problems for the interpretation of ancient physiologies which may have used the CODH/ACS system. Paleoenzymological recovery of predicted ancient homologs will allow an unprecedented look at the kinetic-isotope evolution of this enzyme family through time, and will be of great usefulness for the interpretation of ancient C, as well as S isotope signals.

***Paleoenzymology of sulfur metabolisms:*** Also in the vein of linking enzyme evolution to isotope fractionation, PI McGlynn leads a project in collaboration with Caltech and University of Seoul Faculty which aims to determine the sulfur isotope fractionation evolutionary biochemistry of the enzymes involved in microbial sulfate reduction. This process is currently the dominant microbial lever on the sulfur cycle in anoxic environments, and relating electron transfer processes, enzyme evolution, and the Earth's sulfur isotope record will allow a much more complete picture of enzyme evolution and the mark it leaves on a planet.

***The microbial phenotype in the presence of ancient enzymes:*** These ELSI projects on ancestral enzyme reconstruction are also accompanied by genomics efforts to re-introduce the ancestral-form enzymes into living organisms, in order to study the phenotype produced with enzymes of different functions or entirely different levels of complexity from modern enzymes. The questions ELSI will pursue for rTCA carbon fixation are how an organism can survive and evolve with cruder enzymes in its deepest core pathways. The questions ELSI will pursue for Calvin-Benson cycle carbon fixation concern the functions of ancient RuBisCO and Carbonic Anhydrase ancestors, which created the evolutionary context for the emergence of a Carbon-fixing function. Carbon fixation using RuBisCO, in particular, has distinctive isotope-fractionation signatures, which depend not only on the central enzymes, but also on Carbon concentration mechanisms that RuBisCO requires to function in different marine or terrestrial contexts in eras with different CO<sub>2</sub> and O<sub>2</sub> levels. In the case of sulfur respiration enzymes, we might be able to trace phenotype evolution of sulfur, sulfate, and even nitrate metabolisms through phenotypic analysis of cells which contain inferred catalytic ancestors.

***Connection to the isotope record and isotope geochemistry:*** With our expertise in protein biochemistry, enzyme evolution, microbial physiology, and frontier level isotope geochemical analyses, ELSI has become poised to be the leader in a field we call **isotope-paleoenzymology**. Through these collaborations, we seek to directly link cellular physiology and individual catalysts (enzymes) to the historical isotope record. The isotope geochemistry group, under the direction of ELSI PIs Yoshida and Ueno, has developed new super-sensitive isotope ratio mass spectrometry techniques which allow direct isotope fractionation factor determination of the enzymes discussed above, as well as their assay through evolutionary time by ancestral state reconstruction analysis. For example, we will be able to assess the evolutionary history of RuBisCO and its associated biochemical proteins by comparing the genomic history of the photosynthetic reaction centers I and II to isotope records in an effort to understand the evolutionary interdependence of innovations that took place in both biochemistry and bioenergetics. Additionally, looking at enzymes involved in sulfur metabolism mentioned above may allow for the ability to link isotope fractionation to the evolution of sulfur respiration.

***Evolution of photosynthesis:*** An additional ELSI project on ancient enzymes and genomes concerns the possible duplication, and the genetic ancestry, of the two photosystems (Photosystems I and II) that work together to provide high-energy charge separations for oxygenic photosynthesis. This work, a specialization of ELSI researcher Yusuke Tsukatani, seeks to determine whether these now-separate photosystems arose through duplication and divergence of ancestral proteins in a single reaction center, and whether they entered the ancestors of cyanobacteria through conserved vertical descent from this

ancestor, or through horizontal transfer from either green-sulfur or purple bacteria, which host them separately today, supporting questions about the rise of oxygen (C7).

### ***Comparative microbial genomics and reconstruction of coupled biochemical and bioenergetics pathways in ancient Earth analog environments***

ELSI researchers are exploring the microbial activity and diversity of early Earth analogs to gain insight into what the first microbial communities were like, and how their collective activities may have forced or contributed to the evolution of the Earth's global elemental cycling. These valuable early Earth analogs provide an environmental context of life as it may have existed in much more reduced environments than are usually accessible on today's Earth.

EON fellow Nancy Merino uses single-cell genomics to understand the interactions of member species in serpentinite-hosted hydrothermal systems as models of the earliest biosphere, doing comparative analysis at the Hakuba-Happo Onsen in Nagano Prefecture and the Cedars in California. This work is in collaboration with the Hadean Bioscience collaboration led by ELSI Fellow Ken Kurokawa. Furthermore, working with ELSI PI McGlynn, Merino has acquired samples suitable for single cell-stable isotope studies using nanoSIMS. Measurements will be conducted in collaboration with Prof. Sano of the University of Tokyo, and these measurements will represent the first direct physiological characterization of Hakuba-Happo onsen.

Other projects concern the microbial activity and ecology of early archaean ocean analogs. Projects led by PI McGlynn at Oku-oku hachikuro Onsen in Akita and in collaboration with Prof. Takashi Kakegawa (Tohoku University), and also at Jinata Onsen are allowing for a picture of possible archaean microbiology to be formed. Geochemically, these hot springs span the likely ocean chemistry from the Archean to the Proterozoic within the spatial confines of meters. At these locations, we are assembling and comparing microbial genomes, especially with relevance to possible early iron, light, and/or hydrogen, iron, and sulfur based metabolisms.

### **C9. How did the thermal evolution of the solid Earth change the ecosystem?**

The long-range evolution of the biosphere as well as the atmosphere and ocean is deeply connected with the thermal evolution of the solid Earth. The links between these categories of evolution have been dramatically reconsidered in recent years. Subject matters that have been revisited include the following: (1) Changes in and evolution of atmospheric composition through volcanic activity and differentiation of the Earth's crust and mantle. (2) Changes in the supracrustal material cycle through plate tectonics, and the link with the emergence of multicellular animals. (3) Effects of the inner core formation and resulting changes in geomagnetic field intensity on the biosphere. (4) True Polar Wander and the Snowball Earth hypothesis (Kirschvink). The driving force in these is related to the differentiation of the solid Earth through the cooling of the Earth. The record of the Earth's history reveals that there were drastic changes in the Sr isotopic composition at 2.1 billion and 600 million years ago. These changes in composition imply the onset of extensive weathering of continents, increase in sedimentary rocks owing to the expanded land areas, and the supply of nutrients to the ocean. The times of the changes appear to coincide with the emergence of eukaryotes and of metazoan animals when the levels of oxygen increased. These coincidences imply possible causal links between these climatic and evolutionary events that may ultimately reflect the thermal evolution of solid Earth. Particularly, the increase in oxygen levels 600 million years ago may have been an inevitable physical trajectory of a cooling planet.

We will clarify how the Earth's core, mantle, and crust differentiated over 4.6 billion years, and especially when radiogenic heat sources were first distributed, and subsequently spread by mantle convection. To do so, we will first determine the physical properties of key substances and their elemental partitioning in the Earth's interior based on the results of experiments under high temperature and pressure in A3 above. Using these parameters, we will simulate the convection of the mantle through time to identify when the convection transformed, and we will identify when the inner core was formed. In addition, we will conduct a dynamo simulation of the metallic core to understand how the geomagnetic field intensity changed by the formation of the inner core.

These simulations should be compared with actual observational evidence. We will measure paleomagnetic intensity of rock specimens from various times in the history of the Earth to study the link between the core evolution and magnetic fields. PI Kirschvink established a method of analyzing measured paleomagnetism as described in A3. PI Maruyama and his team discovered that continental growth was episodic throughout the history of the Earth (Rino et al., 2008). Igneous activity is closely linked to the thermal evolution of the solid Earth. Comparing the implied solid Earth evolution with the surface environmental changes shown in the study of drill core samples will establish links between the Earth's

interior and surface environment. In regard to direct influence of environmental changes on the biosphere, we will examine changes in composition of the atmosphere and ocean by extending the method described in B4. To study links between plate tectonics and the biosphere, we will conduct a geochemical analysis and model biogeochemical cycling of key elements not only within biosphere but also include crust and mantle in a longer timescale. PI Maruyama and his team studied changes in temperature and pressure of subducted plates in regional metamorphic belts, and arrived at the conclusion that, as the Earth cooled, subducted oceanic plates carried water to the mantle, and the total quantity of seawater decreased thereafter (Maruyama et al., 1996; 1997; Maruyama and Liou, 2005). The decrease in seawater exposed vast areas of continent above sea surface. The denudation of the continents increased the supply of nutrients to the ocean and substantial organic carbon burial into sediments, possibly triggering the elevation of oxygen levels that may have triggered emergence of animals at 600 million years ago.

Focusing on the times 600 million years ago, our G-COE project has carried out continental drilling over 10 sites and performed thorough geochemical and paleontological analyses (e.g., Sawaki et al., 2010). In this project, we will focus on even earlier times to obtain pristine drill core samples of critical events.

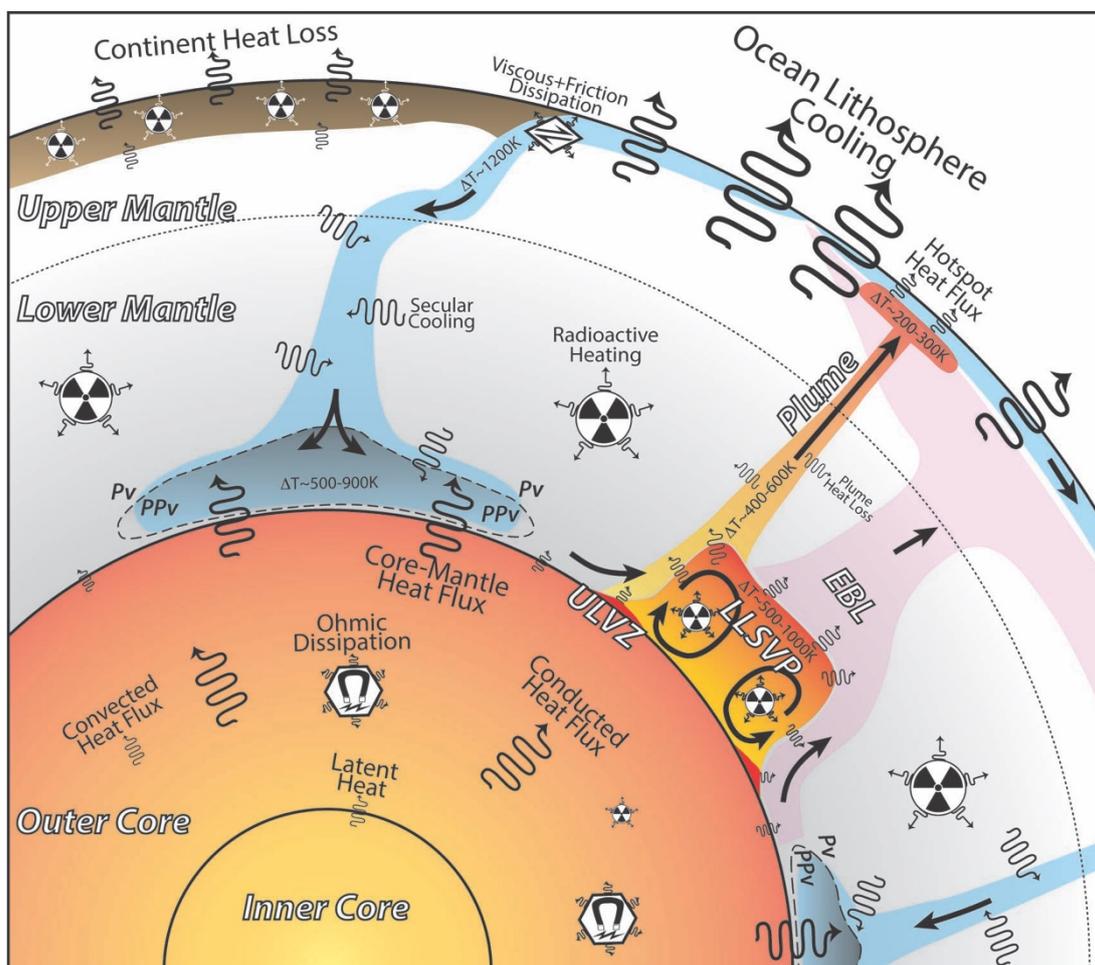


Figure 8. The evolution of the Earth's interior should have affected surface environments through enhancement of geomagnetic field, landmass, and sedimentary rocks. (related to question C9).

### D10. How unique is our planet?

Fundamental questions about the formation and evolution of habitable terrestrial planets such as "What is the diversity of terrestrial planets, and how does Earth fit in?" and "What is special about life on Earth?" can now be addressed in quantitative ways based on actual observations, experiments and simulations. We assemble the ever-growing data of extrasolar planets (more than 4000 exoplanets, and observed detailed characteristics of some planets) and our solar system bodies (8 planets and the other small bodies), and we clarify both universal and unique aspects of our Earth (Comparative Planetology). Then, we find conditions for life to emerge and its subsequent long-term evolution, and identify how these conditions

can be reproduced in the “Comparative Planetology” framework. We will review and synthesize results concerning the composition and the amount of the atmosphere, the amount of ocean (ocean to land ratio), the effect of the large moon(s), the possible onset of plate tectonics, generation of a magnetic field, evolution of planetary interior, and positional relationships between planets and the Galaxy evolution. We promote the study of the Earth based on comparison with its closest neighbors and more distant cousins, using both Earth specificity and planetary diversity to advance towards a better understanding of planets as a whole. This integrated knowledge will be able to be used for narrowing down the targets that potentially host extraterrestrial life, which is related to D11. In future JAXA’s planetary exploration missions after Hayabusa-2 and MMX missions, and in future large telescopes such as TMT and E-ELT, we will actively and scientifically collaborate with JAXA and NAOJ.

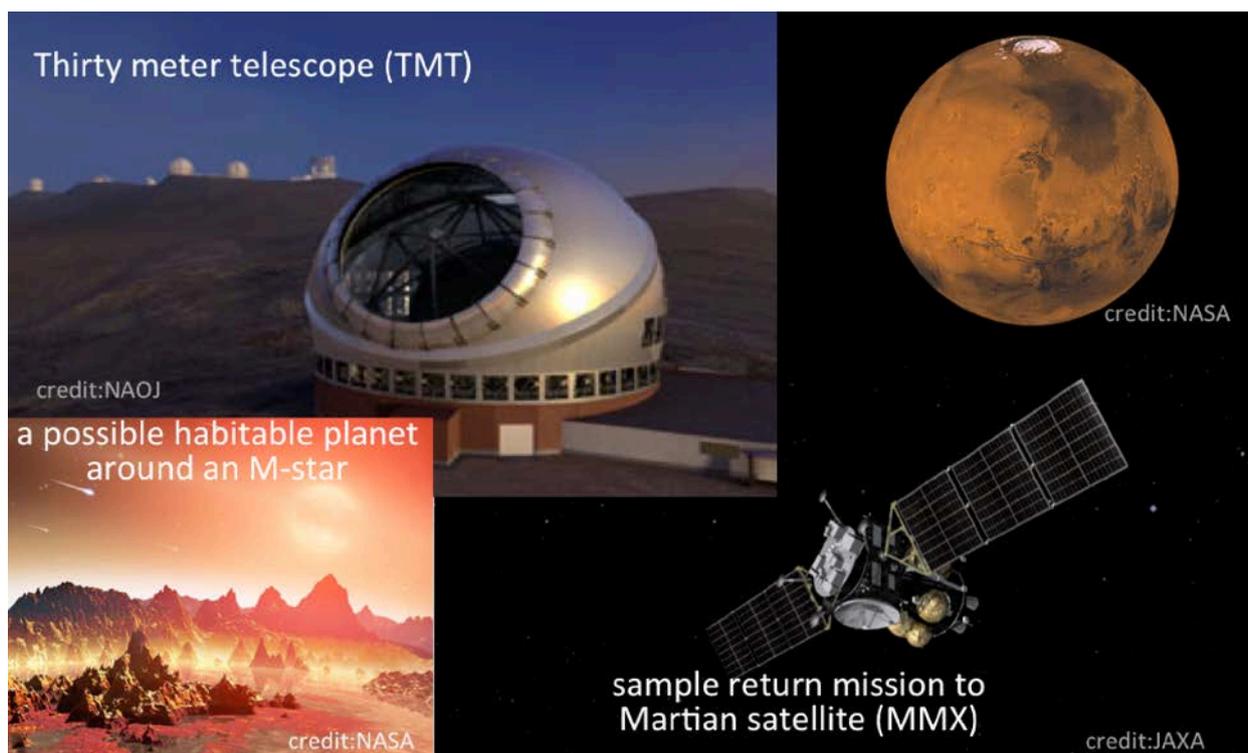


Figure 9. We will participate in future space exploration projects (such as the mission to a Martian satellite by JAXA) as well as in science plans to look for biomarkers by remote sensing of terrestrial planets outside the solar system using a next-generation large telescope, TMT, which Japan participates in (related to questions **D10** & **D11**).

### **D11. How should we search for extraterrestrial life?**

The research outcomes from the above A to C will be utilized for remote sensing observation by ground telescopes and space exploration missions, particularly for search for biosignatures of extra-solar Earth-like planets in the habitable zones and on-going Hayabusa-2 and scheduled MMX missions.

Spectroscopic observation of the atmosphere of extra-solar terrestrial planets in habitable zones will be available by next-generation large telescopes, TMT and E-ELT. Since National Astronomical Observatory Japan is a formal partner for TMT, Japan ABC (AstroBiology Center) is focusing on instrument development for TMT. We will try to establish more generalized biology that can be applied for remote sensing of biosignatures on these planets and make clear what can be biosignatures and how to observe them, in collaboration with Japan ABC.

As for a discussion of life diversity in the universe, we will link data on life in extreme environmental conditions on the Earth and those from searches for extraterrestrial life with data from geology, discussions of planetary condition based on the state-of-art planet formation theory, the history of the Earth, and Earth's interior physics. To be more specific, as case studies, we will consider the possibility of existence of life on celestial bodies with subsurface oceans of icy satellites in the solar system and planets in habitable zones around M-type stars. Compared to our sun, M-type stars are so faint that the habitable zones are very close to the central stars. Owing to tidal actions, the planet's rotation and revolution should be

synchronized, with one particular side facing the central star. The planets receive intense X-rays and ultraviolet fluxes owing to its proximity to the central star. These planets, although they are in habitable zones, have environments that differ significantly from that of the Earth. These discussions are also applied to discussions on possible life in deep subsurface ocean of icy satellites of Jupiter and Saturn (Europa and Enceladus).

Commitments to sample return missions are also important roles of ELSI.

JAXA's Hayabusa-2 will return samples from a primitive C-type asteroid (Ryugu) in 2020. Water and organic matters are expected to be found in the samples. We focus on developing scientific scenarios, rather than mission details. We use the renovated planet formation model to interpret the sample analysis results and consider their implications for prebiotic chemistry.

The sample return mission from a Martian satellite (Phobos or Deimos), called MMX (Martian Moons eXplorer), by JAXA will be launched in 2024. MMX will give important clues not only on the origin of Martian satellites but also on primitive Martian surface environments. Because Phobos and Deimos closely orbit Mars, debris generated by early impacts to Mars may be injected to the surface of these satellites and the debris from early Mars may also be found in the samples. Using our findings of more general biology on early Earth, we will also discuss early Mars as another suitable site of origin of (primitive) life.

## **D12. What principles lead to life in a planetary context?**

ELSI research will focus on the aspects of life for which theoretical problems couple most directly to the geological, chemical, and microbial data and models that are the Institute's unique strength. We will advance methods to reason about complex chemical systems (B5), to understand how biochemistry is related in detail to geochemical conditions (B6, C7), and to understand why motifs such as cellular and genomic individuality are so fundamental to biological organization, and how living systems embody models of their world and use these to become partly independent of its constraints. Specific areas of specialization include: 1) advanced computational methods to map the large combinatorial spaces of both molecules and possible reaction systems; 2) efforts to understand which aspects of life are robust due to familiar principles of irreversibility in reaction-diffusion systems, and which require new physics that includes mesoscale fluctuation and irreversibility; 3) the nature of concepts such as memory, individuality, agency, and cognition, which underlie both the existence and autonomy of cells and higher organisms, and thereby enable the Darwinian dynamics of heredity and selection by which they evolve. The EON program at ELSI has been a particularly valuable network through which to identify and recruit talented scientists working in these areas.

### ***Advanced Computational Chemistry***

Many core problems in pre-biotic chemistry require the ability to assemble constraints on molecular form, or the generating mechanisms of reactions, into complex networks, and then to search and reason systematically about the properties of these networks. To address these needs, we are developing new computational chemistry tools in multiple parallel tracks. Our first program, directed by James Cleaves, concerns the combinatorial spaces of molecules. Our second program, supervised by PI Eric Smith, centers around new techniques of graph-rewrite-grammars for representing large reaction networks.

In one example of the way combinatorial computational chemistry can help show whether biological properties are necessary or frozen accidents, Cleaves et al. generated an exhaustive set of amino acids comparable to the biological inventory, and used this to compare chemical properties provided by the 20 genetically encoded amino acids with those provided by randomly chosen alternative sets. They found that the biological set may represent a largely global optimum, reflecting strong natural selection (Ilardo et al., 2015), and suggesting that independent instances of life would employ similar sets. Other projects enumerate lists of alternatives to RNA in order to understand what makes RNA unique (Cleaves et al., 2015; Wang et al., 2016), and to deduce what types of other molecules could have carried memory in sequence information before RNA and DNA appeared (Guttenberg et al., 2015).

ELSI's second program in computational chemistry centers on the use of graph re-write rules to abstract reaction mechanisms so that they can be applied in an unlimited range of molecular contexts. From graphical representation of reaction patterns, molecular reaction networks of arbitrary size may be generated recursively from a few starting molecules. All atom positions and bond configurations may be tracked through the entire network, enabling detailed comparison with position-specific isotope signatures measured in the group of ELSI PI Yoshida. EON fellow Jakob Andersen is a world leader in chemical graph-grammar methods (Andersen et al., 2012; 2014a, b), who has modeled multiple large systems of pre-biotic interest, including the formose network that produces sugars including ribose (Andersen et al., 2013a), and the Hydrogen Cyanide polymerization and hydrolysis network (Andersen et al., 2013b; 2015),

which produces nucleobases. Extensions of these methods at ELSI will introduce stereochemistry and catalysis by metal centers, enabling us to explore a class of reactions widely believed to be fundamental to the emergence of metabolism from geochemistry (Braakman and Smith, 2014; Smith and Morowitz, 2015).

A third, independent approach to overcome the combinatorial complexity of the constraints imposed by chemical consistency, using biological models of parallel signaling systems, is pursued by ELSI Fellow Masashi Aono. Aono and others developed a heuristic search model to solve various constraint satisfaction problems and demonstrated the capacity of the model to simulate unknown chemical reaction kinetics in a semi-quantitative and resource-saving manner (Aono et al., 2015; Aono and Wakabayashi, 2015).

Other research at ELSI seeks to understand the dynamics of complex chemical systems at a more abstract level, through the construction of computational “toy models” that exhibit some features of organic chemistry without reproducing every detail. The aim of this research is not to model one specific chemical system, but to understand what kinds of chemical properties and driving forces are needed for the “messiness” of prebiotic chemistry to transition into ordered states, and for phenomena such as information transmission and natural selection to arise. Current ELSI researchers include PI Eric Smith and researchers Nathaniel Virgo and Olaf Witkowski.

### ***Nonequilibrium physical foundations***

The hypothesis that life on Earth was inevitable, driven into existence by thermodynamic stresses, has existed in its modern form for about 40 years, and has been elaborated by many authors (for summary and bibliography, see Smith and Morowitz, 2015). Yet it is not known whether this hypothesis is correct, or even whether it requires only classical thermodynamics or also additional microscale and mesoscale physics. A multi-part theoretical program under the direction of PI Smith is addressing these questions. As an example of current research on this problem, Stuart Bartlett (joint with NASA JPL and one of the founders of the hydrothermal Origin of Life scenario, Michael Russell (Russell et al., 1998; Russell et al., 2014)), is exploring the limitations of classical theories such as Maximum Entropy Production (Kondepudi and Prigogine, 1998), and the relations between thermal and chemical pattern-formation in vent environments, in relation to the emergence of a proto-metabolism.

### ***Memory, individuality, agency, cognition***

A widely known NASA definition of life — *“a self-sustaining chemical system capable of Darwinian evolution”* — contains no reference to almost any of the specific architectures that are fundamental to biochemistry, molecular biology, cells, or organisms on Earth. ELSI PI Piet Hut has advanced a complementary definition of Origins that abstracts the key features of life omitted in the NASA formulation: *“The Origin of Life was the spontaneous emergence of autonomous agents in a complex system.”* Projects supervised by Hut seek to understand how ordinary matter, driven by the stress of thermodynamic disequilibrium, is forced into architectures that take on the abstract properties of memory, individuality, agency, and cognition. Nathaniel Virgo and Nicholas Guttenberg developed a dynamical “reservoir” model to show how hereditary memory enabling evolution could have arisen from bulk chemical systems before genomic heredity was possible (Virgo and Guttenberg, 2015). Other work by Virgo, relating the topology of a reaction network system to its dynamics, shows how autocatalysis can arise in simple chemistries where it provides focusing and amplification (Virgo et al., 2016). Hut and Olaf Witkowski, jointly with Araya Brain Imaging, are studying the origin of autonomy and how it can lead to the most basic capacities for cognition, the fundamental property of life to categorize its environments and respond in ways that reflect its adaptedness.

### ***Comparative emergence as a new fusion domain***

A common theme in many of the above projects linking Earth and Life is the emergence of new hierarchical levels with properties different from any of those of their components. A second motif shared by these projects is the many advanced methods of comparative analysis, in domains from planetology to biology. Although there is only one Earth harboring Life that we know, there is enough internal diversity in both systems that comparative analysis can be very informative about law and causation; our science is not limited by a statistic of “ $n = 1$ ” in the way that is sometimes claimed. We propose to create a new fusion domain by applying comparative analysis to the origin of novel structures and functions across the Earth and Life sciences, to understand common aspects of the emergence of novelty across cases. We refer to this study with the term “comparative emergence”.

### 3. Management

#### i) Center director

- Provide the name of the center director, his/her age (as of 1 April 2017), specialties, and brief career profile(within 5 lines).
- If there is a plan to change the center director, how does the new center director intend to construct the center and what is his/her vision of objectives to be achieved? Provide a synopsis written by the new center director (free format).

##### **Name of Center Director:**

Name: **Kei Hirose**  
Age: 49

Director of the Earth-Life Science Institute and Professor at Tokyo Institute of Technology. A high-pressure geoscientist who has won many awards: 2006 Inoue Prize, 2007 Japan IBM Science Prize, 2007 Thomson Scientific Research Front Award, 2011 Japan Academy Prize, 2011 Science Innovation Award – Ringwood medal from the European Association of Geochemistry, and most recently, 2016 Fujihara Award from the Fujihara Foundation of Science.

#### ii) Administrative director

- Provide the name of the administrative director, his/her age (as of 1 April 2017), and his/her brief career profile(within 5 lines).

##### **Name of Administrative Director:**

Name: **Takashi Sakurai**  
Age: 66

B.S. in physics, 1973, Tokyo Institute of Technology; D.Sc. in astronomy, 1978, University of Tokyo. He was at the University of Tokyo in 1978-1992, then moved to the National Astronomical Observatory of Japan (1992-2016). His research field is solar physics, and was awarded the JpGU fellow in 2014. He was appointed as administrative director of ELSI in 2016 April.

#### iii) Composition of administrative staff

- Concretely describe how the administrative staff is organized.

Under the leadership of the center director, ELSI has built a comfortable research and living environment particularly for foreign researchers so that they can concentrate on their research. An administrative director with rich experience in research, internationalization and management oversees ELSI's operational and administrative division which is as follows.

- Administrative director, administrative vice director
- General affairs: 1 chief and 1 staff
- Financial affairs: 1 chief and 1 staff
- Life advisor: 1 staff
- Secretaries' office: 7 staff
- Public relations office: 1 chief and 1 staff
- Computer network system: 1 staff
- Coordinator of international initiatives: 1 staff
- University research administrators (assistant directors): 2 staff

##### Key areas of responsibilities:

- General affairs and financial affairs handle our institutional rules, labor management, financial accounting and budgeting, procurement, travel expenses, management of items, facilities, health and safety, and liaisons with the rest of Tokyo Tech etc.
- The life advisor provides foreign researchers and their families with assistance and language support to help them adapt to life in Japan. For example. immigration, housing, child daycare services, Japanese classes and more.
- The secretaries' office is in charge of administrative tasks for the directors and researchers. Their role includes hosting international symposia and workshops.

- The public relations office is responsible for promotional and outreach activity, such as sending out information via our website, social media and printed materials, building media relations, holding public lectures and outreach events, and welcoming visitors from high-schools and overseas research institutions, in order to introduce mission and activities of ELSI and the entire WPI program.
- The computer network system supports information and communication technology, the ELSI network, and provides common computing resources and information security.
- The coordinator of international initiatives plays an active role in seeking research funds and donations from external foundations and enterprises. She offers assistance with recruitment of non-Japanese scientists.
- The university research administrators or assistant directors serve to coordinate between administrators and researchers, assist in handling grant proposals and procurement.

Administrative staff members are fluent in English and possess rich administrative and technical experiences, which helps the director to make decisions.

The secretaries' office was centralized in one office so that secretaries can accumulate and share useful information and know-how among themselves. Upon researchers' request, a one-stop research support system has been developed and a contact person was assigned to each researcher.

The administrators and secretaries keep each other up to date and exchange information regularly.

In addition, Tokyo Tech research strategy office, international office and research administration center, and other divisions of the University provide enough support to ELSI.

#### **iv) Decision-making system**

- Concretely describe the center's decision-making system.

The center director will have the authority to make all decisions except for those concerning the final selection/removal of the center director himself. The responsibilities of the center director include the operation and management of the institute, fully assisted by the administrative director. This will enable a flexible and fast decision-making system.

Based on advice from the directors' office meetings, steering committee meetings and related committee meetings, the director makes administrative decisions on general issues concerning the institute. One of the vice directors is responsible for the secretaries' office and research promotion, and another vice director (foreigner) leads internationalization such as the recruitment of young researchers, visitors and students from abroad.

The directors' office consists of the director, two vice directors, the administrative director, two assistant directors and the coordinator of international initiatives. They hold a regular weekly meeting to deliberate over the latest and most important issues. This enables them to give unified instructions to the committees as well as to ensure the institute runs smoothly.

ELSI has a monthly steering committee consisting of the center director as a chair person, two vice directors, the administrative director, and two other principal investigators, to assist the center director in making decisions on a wide range of matters, such as negotiation with the host university, internal adjustment of policies, and discussions of research environments and personal affairs. In order to promptly share tasks and information, assistant directors, administrative staff above chief-level and secretaries attends the steering committee meeting.

ELSI organized several specialized committees to take action in regards to its smooth running and fusion of interdisciplinary studies. For example, Scientific Committee supports the director to set the strategic direction of science and promote research interactions.

The international advisory board consists of top scientists including non-Japanese, and the board members offer advice from an international perspective. ELSI director receives advice from them, but makes the final decisions by himself.

#### **v) Allocation of authority between the center director and the host institution's side**

- Concretely describe how authority is allocated between the center director and the host institution's side.

While the president of Tokyo Tech has the authority concerning the final selection/removal of the center director, the center director will be empowered to regulate the rest of the management and operations concerning the center. Opinions are exchanged once a month with the university executives (president, executive vice president for research, executive vice director for general affairs and finance)

and center director in order to maintain close coordination between Tokyo Tech and ELSI.

#### 4. Researchers and other center staffs, satellites, partner institutions

##### i) The “core” to be established within the host institution

##### a) Principal Investigators (full professors, associate professors or other researchers of comparable standing)

	numbers		
	At beginning	As of April, 2017	Final goal (Date: October, 2019)
Researchers from within the host institution	6	12	12
Foreign researchers invited from abroad	3	2	3
Researchers invited from other Japanese institutions	4	1	1
Total principal investigators	13	15	16

- Describe the concrete plan to achieve final staffing goal, including steps and timetables.
- Attach a list of principal investigators using the Appendix. Place an asterisk (\*) by names of the investigators considered to be ranked among the world's top researchers. Describe the policy and strategy for inviting the PIs who are to be included after 1 April 2017.

Since its inception, ELSI has strategically recruited new PIs from abroad and other Japanese institutions and built up a superb lineup of 15 PIs including one female non-Japanese PI and eight non-Japanese PIs. 3 PIs work in three Satellite Centers at IAS, Harvard University, and Ehime University. Although the current set of PIs cover top-rate scientists from a range of diverse disciplines to achieve our scientific missions, ELSI is always looking for more talents, especially in younger generations, to think ahead toward the future of ELSI.

##### b) Total members

	Numbers		
	At beginning	At end of FY 2016	Final goal (Date: October, 2019)
Researchers	23 <3,13%> [0,0%]	63 <29,46%> [11,17%]	70 <35,50%> [16,23%]
Principal investigators	13 <3,23%> [0,0%]	19 <8,42%> [1,5%]	16 <9,56%> [1,6%]
Other researchers	10 <0,0%> [0,0%]	44 <21,48%> [10,23%]	54 <27,50%> [15,28%]
Research support staffs	0	29	29

Administrative staffs	5	25	25
Total number of people who form the "core" of the research center	28	117	124

- Enter the total number of people in the columns above. In the "Researchers" column, put the number and percentage of overseas researchers in the < > brackets and the number and percentage of female researchers in the [ ] brackets.
- Enter matters warranting special mention, such as concrete plans for achieving the Center's goals, established schedules for employing the main researchers, particularly principal investigators.

## ii) Collaboration with other institutions

- If the "core" forms linkages with other institutions, domestic and/or foreign, by establishing satellite functions, Provide the name of the partner institution(s), and describe the role of the satellite functions, personnel composition and structure, and collaborative framework between the host institution and the said partner institutions (e.g., contracts to be concluded, scheme for resource transfer).
- If some of the principal investigators will be stationed at satellites, attach a list of these principal investigators and the name of their satellite organizations using the Appendix.
- If the "core" forms organic linkages with other institutions, domestic and/or foreign, without establishing satellite functions, provide the names of the partner institutions and describe their roles and linkages within the center project.

## 1) Satellite Center

ELSI will have four Satellite Centers, i) at the Geodynamics Research Center, Ehime University, (ii) at the Department of Earth and Planetary Science at the University of Tokyo, (iii) at the Interdisciplinary Program, Institute for Advanced Study in Princeton, and (iv) at the Origin of Life Initiative, Harvard University. Each satellite function is as follows.

### Geodynamics Research Center (GRC), Ehime University

GRC has shown globally leading research results in the fields of deep Earth science. Prof. Tetsuo Irifune will join ELSI as a Principal Investigator and Satellite Director. Some more GRC members (including one female scientist) will also join this Satellite Center.

The main role of this Satellite Center at Ehime University is to conduct research on the origin and evolution of the solid Earth, primarily based on the high-pressure/high-temperature experiments using multi-anvil apparatus (large-volume press). Such multi-anvil experiments have a great advantage in controlling sample temperature over experiments by other techniques such as a laser-heated diamond-anvil cell, although the experimental pressure-temperature range is limited. The combination of both diamond-anvil experiments (K. Hirose at Tokyo Tech) and multi-anvil experiments (T. Irifune at Ehime Univ.) would provide the best answers to questions on the deep Earth structure and dynamics.

### Department of Earth and Planetary Science, University of Tokyo (EPS/U.Tokyo)

In April 2017, ELSI will launch a new satellite in the Department of Earth and Planetary Science (EPS) at the University of Tokyo. The Institute Director Hirose will promote his own research on the formation and early evolution of our planet in collaboration with experts in geochemistry and thermal evolution modeling at the EPS/U.Tokyo and lead collaborative research between ELSI and EPS/U.Tokyo. In order to facilitate the launch of this new satellite, the Institute Director Hirose will be cross-appointed by the University of Tokyo as of April 2017 and will work 20% of time at the EPS/U.Tokyo. The EPS/U.Tokyo has strong research groups in astrobiology, planetary science, solar system exploration, early Earth geochemistry, and the evolution of life. Importantly, their research is complementary to that of current ELSI members. Director Hirose will lead joint research between ELSI and the EPS/U.Tokyo satellite center in the study of the formation, evolution, and habitability of planets in solar and extrasolar systems and the study of geology, geochemistry, and life on the early Earth. Such collaboration will be built through hiring Research Scientists who work at both campuses, co-hosting visitors, and co-organizing international workshops.

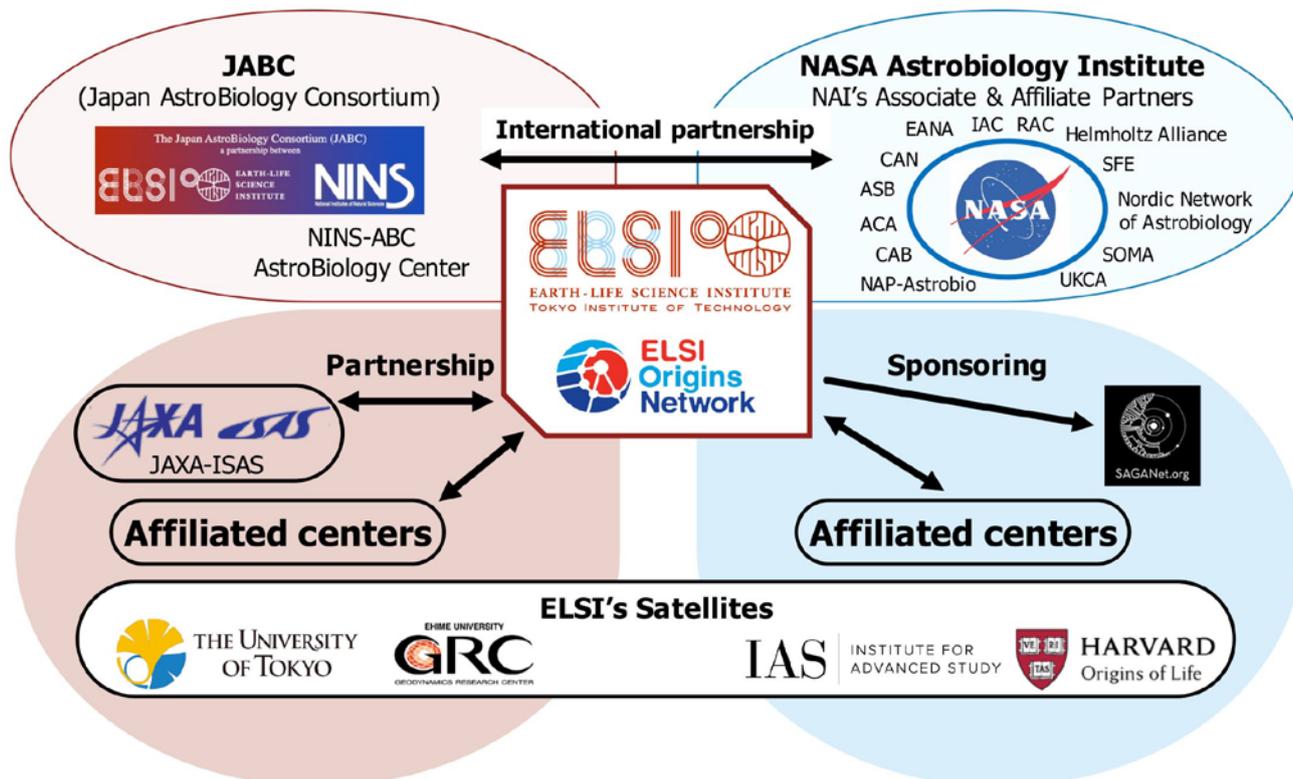
### Interdisciplinary Program, Institute for Advanced Study (IAS) in Princeton

Prof. Piet Hut is based at the IAS in Princeton. He will divide his time between Tokyo Tech and Princeton, half and half. During his stay at Princeton, the Institute for Advanced Study will host scientists from ELSI and EON. The IAS is, of course, a world-leading research institute, always hosting more than a hundred

visitors from around the world. This is an ideal place for ELSI and EON scientists to exchange ideas with other top-class scientists and to establish their own personal connections.

### Origin of Life Initiative, Harvard University

Prof. Jack Szostak will participate as a Principal Investigator and a Satellite Director on behalf of Harvard University Origin of Life Initiative. He is a world-leading scientist in synthetic biology. ELSI and Harvard satellite center will exchange young scientists to explore questions about the origin of life, based on new findings about the early Earth environments, which are under investigation at ELSI.



**Japan**

**International**

Figure 10. Collaboration with domestic and overseas research institutes, including the Satellite Centers

- If the “core” forms organic linkages with other institutions, domestic and/or foreign, without establishing satellite functions, provide the name of the partner institutions and describe their roles and linkages within the center project.

### 2) Affiliated centers

ELSI will have strong connections with domestic and overseas research institutions, such as (i) Japan Agency for Marine Science and Technology (JAMSTEC), (ii) Harvard University, (iii) California Institute of Technology and (iv) Columbia University. ELSI concluded a coordination agreement with JAXA (Japan Aerospace Exploration Agency)/ISAS (Institute of Space and Astronautical Science). Additionally, ELSI has been collaborating with affiliated centers abroad on the basis of the ELSI Origins Network (EON) project funded by the John Templeton Foundation, with which we hire joint postdocs who spend half time at ELSI and the other half there (Figure 13). ELSI promotes collaborative research with these institutions by exchanging people and ideas.

### 5. Research Environment

- Concretely describe measures to be taken to satisfy each of the requirements outlined below, including steps and timetables.

- Provide an environment in which researchers can devote themselves exclusively to their research, by exempting them from other duties and providing them with adequate staff support to handle paperwork and other administrative functions.**

The Earth-Life Science Institute (ELSI) will provide the best environment for researchers to concentrate on research. PIs (principle investigators), specially appointed associate / assistant professors and post-docs will work together and pursue their research interests freely with loose connection to a specific group. A few university research administrators with academic backgrounds provide additional support in order for researchers to avoid miscellaneous tasks which are non-essential to their research. They also help non-Japanese researchers in general ways, including offering assistance with writing a proposal, communicating with external Japanese scientists, etc. PIs joining from Tokyo Tech have been reassigned as Professors of ELSI, which grants them a reduction in non-research responsibilities. They must at least be exempted from the duty of teaching undergraduate students.

The center director is responsible for minimizing the administrative work of all researchers at the center. For this purpose, a very efficient research-oriented administrative division has been created through several unique systems. Each administrator will be evaluated and given incentives, similarly to scientists. The center holds a regular event to inform administrators of the center's latest research results, which leads to smooth communications between researchers and administrators and more importantly motivates the administrators to work for the research.

**ii) Provide startup research funding as necessary to ensure that top-caliber researchers invited to the center do not upon arrival lose momentum in vigorously pursuing their work out of concern over the need to apply immediately for competitive grants.**

Each PI invited from overseas will be granted JPY5 to 10 million, depending on whether they conduct theoretical or experimental work, as start-up funding for his/her research project. Further support will possibly be given at the discretion of the center director, until he/she obtains external funds based on the discussion with the center director. The center will provide non-Japanese researchers with a full range of support to acquire competitive funds in Japan.

The director's fund will be utilized to encourage interdisciplinary concepts borne out of young researchers' free and flexible ideas or from discussions between researchers with different backgrounds. The fund is meant to support feasibility studies and then to acquire competitive funds. The center director receives and reviews joint proposals about twice a year, in the spring and fall. The center keeps track of their progress and will determine how the internal funding system should be managed in later stages.

**iii) As a rule, fill postdoctoral positions through open international solicitations.**

Through open international solicitations, the center hires three ranks of researchers besides PIs: 1) post docs, 2) specially appointed assistant professors, and 3) specially appointed associate professors. Their expertise and strengths should fit within ELSI's scientific interests and goals, and they should be open-minded to collaborate with other researchers from diverse backgrounds both in and outside of ELSI. Young researchers have more freedom in their research with only loose connections to specific groups. Their academic independence was guaranteed in ELSI's open and flat research structure that departed from the conventional one in which young researchers assisted PIs under the PI's leadership. Instead, young researchers at ELSI form their own networks and seek advice and cooperation from various PIs and researchers with whom young researchers' interests align. Such dynamic collaboration and fusion among researchers will be encouraged, and the research structure will be reviewed and improved.

Now that ELSI has recruited top scientists and their research environments are settled, the strategic addition of new members will speed up collaborative research projects, leading to more results.

**iv) Establish English as the primary language for work-related communication, and appoint administrative personnel who can facilitate the use of English in the work process.**

The official language must be English for non-Japanese and Japanese alike. Every document will be written in English. A few officers of Tokyo Tech who can use English will be assigned to the center as a priority. We will also have excellent English-speaking staff members from the outside, and we will actively encourage the employment of staff, Japanese and non-Japanese, with international experience.

- v) **Adopt a rigorous system for evaluating research and a system of merit-based compensation. (For example, institute a merit-based annual salary system primarily for researchers from outside the host institution. As a basic rule, the salaries of researchers who were already employed at the host institution prior to the centers' establishment are to be paid by the host institution.)**

The research activity by each scientist will be evaluated annually. The evaluation process has been restructured into several layers. Firstly researchers review their activities and submit a report on publications in academic journals, the scientific merit of his/her research, their contribution to ELSI's overall activities and the acquisition of external competitive funds. Then newly assigned mentors add statements and forward the assessment results to senior PIs and Director's office. For outstanding research outcomes or contributions, the center will provide better research environments (space, financial support etc) and treatment (salary raise and extension of contract) as incentives. While every researcher is to get feedback on the results, it will be important for researchers who need assistance can receive suggestions for improvement, to be discussed with their mentors and collaboratively monitored throughout the year. In addition, the directors regularly communicate with researchers, in order to exchange opinions on and to discuss future directions for his or her research.

Administrator will be evaluated and given incentives for notable achievements.

- vi) **Provide equipment and facilities, including laboratory space, appropriate to a top world-level research center.**

Tokyo Tech has secured sufficient research space (about 1500 m<sup>2</sup> from the start and an additional area of approximately 5000 m<sup>2</sup> by 2015) for the center at the Ookayama campus, close to the building of the department of Earth and planetary sciences. In addition to research space (offices, laboratories), we will keep a common room to promote internal communications, which is key for interdisciplinary studies. Both researchers and administrators gather in this room for their short break and for daily and weekly events.

The access to research equipments, in particular to large scale parallel computers for simulations, is abundant. The computer center of Tokyo Tech (GSIC) has the most advanced supercomputer TSUBAME among research institutes in Japan. In addition, GRAPE series of custom-built supercomputers, developed by J. Makino's group, will be accessible to researchers of the center. Also, 10-Petaflops K computer and its successor, the post-K supercomputer, as well as other supercomputers in national research institutes, including the National Astronomical Observatory, JAXA and JAMSTEC are accessible.

- vii) **Hold international research conferences or symposiums regularly (at least once a year) to bring the world's leading researchers together at the center.**

An international symposium will be held annually. They will cover a wide range of topics, with different clear-cut key concepts in each year, based on original research at the center. World-leading scientists and young active researchers will be invited from abroad with and without travel support. Other relatively small workshops on specific hot topics and interdisciplinary topics will be held several times each year.

- viii) **Other measures to ensure that top-caliber researchers from around the world can comfortably devote themselves to their research in a competitive international environment, if any.**

Living conditions will probably be the biggest concern for most non-Japanese scientists. To best serve them and their families, the center will assign a "life adviser" to each family before they even move to Japan. This adviser will guide them through all the difficult processes and will always be available to advise on subjects such as visas, schools, bank accounts, special diets, garbage, transportation, taxes, pensions, etc. The adviser essentially acts as a personal assistant for non-Japanese scientists when needed. Tokyo Tech has an accommodation facility called the 100th Anniversary International House with 100 single rooms and 20 family rooms at Ookayama campus. It can be used temporarily by non-Japanese scientists

and their families until they find a place to live elsewhere.

Another challenge for non-Japanese scientists will be the acquisition of external funds for their research. ELSI's university research administrators will be heavily involved in their preparation of proposals. Additionally, the university's research administration center, research promotion department and international affairs department will support non-Japanese scientists in acquiring competitive funds.

## 6. Indicators for evaluating a center's global standing

• Describe concretely the following points.

### i) Criteria and methods to be used for evaluating the center's global standing in the subject field

Evaluation of a "globally visible" research center requires a comprehensive assessment with consideration of various criteria such as levels of research activities and recognition of the institute and its researchers. Specific evaluation indicators include 1) the number and quality of publications, number of conference presentations, number of scientific events hosted, and acquisition of research funding for research activities and 2) degree of international research cooperation, number of visitors, and academic awards for recognition of the institute and its researchers.

It is equally important to carefully assess the progress of efforts to promote interdisciplinary research and to create a new research domain.

### ii) Results of current assessment made using said criteria and methods

#### Current assessment of research activities

8 out of 15 PIs in ELSI have "h-index" higher than 35. It is clear that ELSI exhibits a strong prospective to stand out globally as top-level research center in the world. Six PIs are under fifty years old and are expected to play leading roles in making major advances in academic activities.

Recent publications (since 2014) of note include the followings:

- Experimental determination of the electrical resistivity of iron at Earth's core conditions (2016) *Nature* 534: 95-98.
- Lunar true polar wander inferred from polar hydrogen (2016) *Nature* 531: 480-484.
- Evidence for global electron transportation into the jovian inner magnetosphere (2014) *Science* 345: 1581-1584.
- Low Core-Mantle Boundary Temperature Inferred from the Solidus of Pyrolite (2014) *Science* 343: 522-525.
- The Charon-forming giant impact as a source of Pluto's dark equatorial regions (2017) *Nature Astronomy* 1: 0031.
- Oligoarginine peptides slow strand annealing and assist non-enzymatic RNA replication (2016) *Nature Chemistry* 8: 915-921.
- Synthesis and stability of xenon oxides  $\text{Xe}_2\text{O}_5$  and  $\text{Xe}_3\text{O}_2$  under pressure (2016) *Nature Chemistry* 8: 784-790.
- Pressure-induced nano-crystallization of silicate garnets from glass (2016) *Nature Communications* 7: 13753.
- A key genetic factor for fucosyllactose utilization affects infant gut microbiota development (2016) *Nature Communications* 7: 11939.
- Carbon-depleted outer core revealed by sound velocity measurements of liquid iron-carbon alloy (2015) *Nature Communications* 6: 8942.
- *Klebsormidium flaccidum* genome reveals primary factors for plant terrestrial adaptation (2014) *Nature Communications* 5: 3978
- Accretion of Phobos and Deimos in an extended debris disc stirred by transient moons (2016) *Nature Geoscience* 9: 581-583.
- Computational support for a pyrolitic lower mantle containing ferric iron (2015) *Nature Geoscience* 8: 556-559.
- Water contents of Earth-mass planets around M dwarfs (2015) *Nature Geoscience* 8: 177-180.
- Stability of hydrous silicate at high pressures and water transport to the deep lower mantle (2014) *Nature Geoscience* 7: 224-227.
- Origin of microbial biomineralization and magnetotaxis during the Archean (2017) *PNAS* DOI:

10.1073/pnas.1614654114

- A virus of hyperthermophilic archaea with a unique architecture among DNA viruses (2016) PNAS 113: 2478-2483.
- On the universal structure of human lexical semantics (2016) PNAS 113: 1766-1771.
- Hadal biosphere: Insight into the microbial ecosystem in the deepest ocean on Earth (2015) PNAS 112: E1230-E1236.
- Oxygenic photosynthesis without galactolipids (2014) PNAS 111: 13571-13575.

ELSI acquired a sum of \$5.5 million USD (approx. 670 million yen) from the John Templeton Foundation (US) for the period from July 2015 to March 2018 and launched a project titled "ELSI Origins Network (EON)". ELSI researchers have been successful in securing research funding. Notably, large KAKENHI funds, such as Grant-in-Aid for Specially Promoted Research, Grant-in-Aid for Scientific Research on Innovative Areas, and Grand-in-Aid for Scientific Research (S), were acquired. These assure continued development of research projects.

### **Recognition of the institute and its researchers**

ELSI's researchers from different generations are held in high esteem at their respective levels. Senior researchers such as PIs have received awards including the Medal of Honor with the Purple Ribbon, the JSPS prizes, and the Fujihara Award. They have also become fellows of notable societies such as the Royal Institute of Navigation. Meanwhile young researchers have also received awards that target young professionals, such as the IUPAC-SOLVAY International Award for Young Chemists.

### **Promotion of interdisciplinary research and creation of a new research domain**

ELSI's efforts to promote interdisciplinary research have been resulting in publications (e.g., Earth Planet. Sci. Lett. 2014 386: 112-125; Astrobiology 2015 15: 430-441; PLoS ONE 2015 10: e0140663; Geochim. Cosmochim. Acta 2016 177: 205-216; Orig. Life Evol. Biosph. 2016 DOI: 10.1007/s11084-016-9516-z). In addition to the institutional activities for scientific discussion, informal discussion groups have been organized voluntarily on various topics, promising more avenues for future interdisciplinary collaborations.

ELSI researchers have conceptualized an idea of a new research domain, which is called "Comparative Emergence," and aim to crystallize this idea of "Comparative Emergence" in the coming five years.

### **iii) Goals to be achieved through the project (at time of final evaluation )**

- a) Establish position as world leader among research institutes in related fields.
- b) Establish a sound financial base by steady acquisition of donations and competitive research funding.
- c) Expand the research community driven by ELSI further and thereby contribute to its diversification and internationalization.
- d) Contribute to the fostering of next-generation researchers and their career development. This will be done by strategically planning the exchange, acquisition, and training of research-related human resources as a hub for idea exchange between researchers, collaborators, and guests.
- e) Create a new fusion domain, Comparative Emergence, by applying modern comparative methods to a systematic study of the emergence of novel structures and functions across Earth and Life sciences.

## **7. Securing research funding**

ELSI has already secured adequate research funds including the Grant-in-Aid for Science Research (KAKENHI), sponsored research funds, collaborative research funds, and university grants/operating subsidies.

ELSI's main source of funding as of FY2016 are funds from the John Templeton foundation based in the U.S., along with large-scale KAKENHI such as Grants-in-Aids for specially promoted research and for scientific research in innovative areas. The research fund from the John Templeton foundation is approximately 5.5 million US dollars in total and has strengthened ELSI's infrastructure to accelerate research related to origins of the Earth and life. In addition, we secured new research funding in FY2016 from NEDO and JSPS's Grant-in-Aids for specially promoted research.

### **Future prospects**

- Describe the concrete prospects for securing resources that match or exceed the project grant.
- Calculate the total amount of research funding (e.g., competitive funding) based on the percentage of time the researchers devote to research activities at the center vis-à-vis the total time they spend conducting research activities. Be sure the prospects are realistically based on the past record.

The following table shows the expected amount of research funds to be obtained annually at ELSI from FY2017 and onwards. This shows that ELSI's capabilities of securing research funding are substantially matched to the requirement by the WPI program

	Research funds to be obtained annually at ELSI from FY2017-2021 (Unit million yen)
Grants-in-Aid for Scientific Research (KAKENHI)	363
Corporate Collaborative Research and Donation for Research, etc.	146
Sponsored Research	18
University Grants / Operating Subsidies	102
<b>Total per fiscal year</b>	<b>629</b>

In order to ensure that the expected funding appears as above, we provide the following structured and strategic efforts to all researchers at ELSI.

- By creating an environment in which all researchers at ELSI can concentrate on research, we will allow them to apply for more competitive funding programs.
- University research administrators will fully assist researchers in acquiring funds. For example, they will arrange grant applications in cooperation with Tokyo Tech's research administration center, research promotion department and international affairs department.
- We will provide comprehensive support to individual investigators in preparing competitive grant proposals to funding agencies in Japan and elsewhere; English and Japanese language editorial support; opportunity identification; training and mentoring of early-career researchers in proposal development; mediating of internal and external collaborations; and rigorous internal review prior to proposal submission.

The center and administrative directors should regularly develop some trend analysis of national policy objectives, related subsidies, and competitive funding programs with the help of the policy making body of Tokyo Institute of Technology. This will ensure a cost-effective approach to support basic funding applications and a more complicated and demanding approach necessary for foundations and other large sources of funds. We will propose new future-oriented large-scale projects to the government on the basis of the trend analysis.

## Others

- Describe activities and initiatives to be taken after project funding ends.
- Describe expected ripple effects ( e.g., how the research center project will have trailblazing components that can be referred to by other departments in the host institution and/or other research institutions when attempting to build their own top world-level research centers ) .
- Describe other important measures to be taken in creating a world premier international research center, if any.

## 1) Activities after the end of the program period

The director will do his utmost to seek donations to ELSI from international nonprofit corporations and from companies with close relations to Tokyo Tech. Major scientific mission of ELSI, questions about the formation of Earth and the origin of life, extraterrestrial life and the space craft "Hayabusa2", and sample return mission to Mars moons are of general interest to the public, which could help us to collect donations.

It is notable that ELSI has received 5.5 million USD (approximately 670 million JPY) from the John Templeton Foundation in the U.S. Using these global funds as a resource, ELSI has further strengthened

its research infrastructure and accelerated scientific investigation to elucidate the origin and evolution of the Earth and life. We have launched the EON (ELSI Origins Network) project where ELSI—as a world-class research hub—develops an international network of researchers across various research fields. Building upon the John Templeton Foundation grant acquisition and the success of EON project, ELSI vigorously seeks for more overseas funding.

Even after the end of the support under the WPI program, the activity of ELSI will continue based on 1) external funds acquired by principal investigators and other members, 2) continued support from the university, and 3) donations.

## **2) Effects on other institutions**

ELSI has already realized the following three goals, which have large ripple effects on institutions nationwide. Our main achievements are as follows:

- i) English-based administration  
Internationalization is one of the important goals of WPI program, and ELSI has introduced following practice
  - English-based administration
  - Merit-based annual salary & incentive award
  - Non-Japanese family support systems will be secured at the center.These serve as role models for other institutions to host researchers from abroad.
- ii) Research-oriented environment  
ELSI has established a highly research-oriented environment. For this purpose,
  - Annual evaluation will be conducted to review the research results of each scientist, the outcome of which will be reflected in the revision of annual salaries and incentive award given by the center director.
  - University research administrators with academic backgrounds will provide a wide range of support to all scientists.
  - PIs from Tokyo Tech will be reassigned to the center and exempt from the duty of teaching undergraduate students.
  - A research-oriented administrative structure has been created and the latest research results are disseminated widely to the administrators (See 3. Management iii) and iv) sections). These unique systems should be helpful for other organizations to become more highly research-oriented.
- iii) ELSI will have stronger connections to the general public.
  - PR chief with academic backgrounds will be in charge of overall promotional and outreach activities.
  - The PR office will organize domestic and overseas press releases, outreach events for the general public including high-schools students, and manage interactive digital communication with various stakeholders, to introduce mission and activities of ELSI and the entire WPI program.
  - Active promotional and outreach activities will make the ELSI and the host institute more visible from the outside, which will be a big advantage for both.

## **3) Other plans important for the establishment of a leading global research center**

- i) World-wide interaction of researchers  
ELSI will continue its efforts to enhance its international status as research hub in related research fields. We will invite top-level professors on sabbatical leave to stay for half a year or a year as well as support short stays by both established and young active scientists. At the same time the center will encourage all scientists including postdocs to stay at overseas partner institutions for a while to exchange ideas and conduct collaborative research. Notably postdocs of the EON project, who spend approximately half of their contract terms at an overseas institution.
- ii) Publication of research findings  
Researchers are strongly encouraged to present research findings and to organize scientific sessions at relevant international conferences. This contributes to the high visibility of ELSI and to attract

researchers and students to ELSI.

iii) Fostering mutual understanding to build synergistic relationships

As a newly-established interdisciplinary research institute, we launched efforts to promote internal communications within ELSI. We have done this by setting up a common room as well as holding daily, weekly, and monthly events following the model of IAS, Princeton, where PI Prof. Piet Hut, one of ELSI PIs, is based. ELSI will continue to offer opportunities to share research targets and to assemble adequately research talents and foster greater mutual understanding among researchers. Such opportunities were developed into several types, ELSI seminars, assemblies and youchien (kindergarten). ELSI seminar is a place for lectures and discussion to which external researchers are invited to speak. ELSI assembly is a science meeting conducted by ELSI researchers, and important issues such as strategic, long-term research objectives are presented and discussed at the initiative of the Science Steering Committee. ELSI also schedules a series of assemblies for ELSI researchers to present their research activities conducted in the last year and latest work-in progress. This helps to share academic interests and to exchange regular feedback with each other. ELSI youchien (youchien is a Japanese word for kindergarten) aims to remove the barrier that exists between different disciplines and sections. Young researchers present their research and specialties to other ELSI members including the administrative staff in simple language.

iv) Reorganization of the research environment

We already have years of experience of interdisciplinary research between geoscience and life science through 21<sup>st</sup>Century COE, G-COE, and WPI programs. Additionally, ELSI has several plans to unite the team in exploring the early Earth environments and the origin of life. First, we have reviewed the research organization and clarified the roles of PIs in response to the midterm evaluation results, and the PIs in a revised organization are expected to play leading roles to achieve these ELSI's scientific mission. Second, the areas of research focus and institutional strategy to achieve these research objectives have been under discussion by the directors, PIs, and young researchers. These efforts generated a shared sense of goals among ELSI researchers, which contributes to further promotion of research interaction and interdisciplinary collaboration.

v) Nurturing the next generation of scientists

ELSI has been making steady progress in contributing to graduate education. Some non-Japanese PIs and Associate Professors are now becoming affiliated with Tokyo Tech Schools and Departments across campus, as main or sub supervisors. ELSI is eager to recruit more prospective PhD students and has succeeded in mentoring students on site. ELSI is expecting more PhD students to join (under application). ELSI researchers will also be assigned to teach classes and be encouraged to set up an international educational program. By doing so, such PhD students and supervisors will simultaneously develop interdisciplinary research both at ELSI and other departments.