

WATER LOSS DURING THE FORMATION AND EVOLUTION PHASES OF ROCKY PLANETS

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Water is an important component for planet habitability. The evolution of planetary water inventories depends on the properties of both stars (type, age) and planets (orbital distance, mass/size, outgassing history), and thus is a complicated problem. Thanks to recent developments in observations and theories, new insights on water loss from rocky planets during the formation and evolution phases have been gained. In this talk we will review these new developments and discuss some large gaps remaining in our understanding on this important problem.



DRIVERS OF SPACE WEATHER FROM EVOLVING YOUNG SUNS: IMPLICATIONS FOR PLANETARY ATMOSPHERES

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Introduction: Planets orbiting young, active stars are embedded in an environment that is far from being as calm as the present solar neighbourhood. They experience the extreme environments of their host stars, which cannot have been without consequences for young stellar systems and the evolution of Earth-like planets to habitable worlds. Stellar Space Weather, triggered by magnetism and the related stellar activity is THE crucial driver of ionization, photodissociation, and chemistry in planetary atmospheres. Winds can compress planetary magnetospheres and even strip away the outer layers of their atmospheres, thus having an enormous impact on the atmospheres and the magnetospheres of surrounding exoplanets.

Stellar magnetic fields and winds also control the spin-down and therefore the activity evolution of a star. Modelling of magnetic fields and their winds is extremely challenging, both from the observational and the theoretical points of view, and only ground breaking advances in observational instrumentation and a deeper theoretical understanding of magnetohydrodynamic processes in stars enable us to model stellar magnetic fields and their winds – and the resulting influence on the atmospheres of surrounding exoplanets – in more and more detail. We address questions on the formation and habitability of environments in young, active stellar/planetary systems. We will discuss how stellar evolutionary aspects in relation to spin-down, activity, magnetic fields and winds influence the erosion of planetary atmospheres in the habitable zone.



THE HABITABLE ZONE AROUND THE SUN AND OTHER STARS

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Introduction: The 'habitable zone', or HZ, is defined as the region around a star within which an Earth-like planet can maintain liquid water on its surface. The term itself comes from Huang [1,2]. In an earlier work [3], Shapley referred to this region as the 'liquid water belt.' Hart [4,5] added the term 'continuously habitable zone', or CHZ, to describe the region that remains habitable (in this same sense) for a finite period of time as the star ages, and brightens, on the main sequence.

The stipulation that the planet in question be 'Earth-like' has led to both confusion and debate. Tasker [6] took this to mean a rocky planet that has exactly the same atmospheric composition as modern Earth. But that interpretation fails to match more modern definitions of the HZ, going back at least to [4]. Hart's model, and all other models since then, included an atmosphere with a variable CO_2 partial pressure which changes in response to the carbonate-silicate cycle. So, to more recent authors [7-9], the term 'Earth-like' implies both the presence of a surface liquid ocean *and* recycling of CO_2 by volcanism and (maybe) plate tectonics. The assumed greenhouse gases are CO_2 and H_2O .

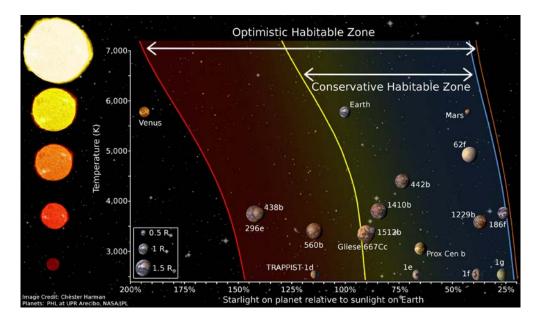


Fig. 1 A modern illustration of the liquid water habitable zone. See text for the definitions of conservative and optimistic HZ boundaries. The locations of Earth, Venus, and Mars are shown, along with a collection of exoplanets identified by Kepler and by ground-based RV and transit surveys. [Figure credit: Chester Harman.]

Importantly, the fact that a planet lies within the HZ of its parent star does *not* imply that the planet is habitable. It merely suggests that it could be, if other factors (e.g., volatile recycling, retention of an atmosphere) are favorable. And, of course, planets (or moons) that lie outside of the HZ could be habitable, especially in their subsurfaces where liquid water might exist. Such life would be difficult to detect remotely, however, as it would not be in direct contact with the planet's atmosphere. The HZ might also be extended outward by the presence of additional greenhouse gases, e.g., H₂, to warm the planet's surface [10]. But such a planet would then not be exactly 'Earth-like'.

HZ boundaries: Fig. 1 shows boundaries of the HZ, as computed from a combination of 1-D and 3-D climate models. The x-axis is chosen to be stellar flux, rather than distance, to emphasize the area that could be habitable. Two different sets of boundaries are drawn: a conservative one and an optimistic one. The conservative limits are those derived from climate models. The inner edge is de-



fined by the occurrence of a runaway greenhouse in which all the planet's water evaporates; the outer edge is defined by the 'maximum greenhouse effect' of CO₂, beyond which CO₂ condensation and an increasingly high planetary albedo combine to keep the surface below freezing. The optimistic limits are defined empirically: The inner edge is based on the observation that Venus has *not* had liquid water on its surface for roughly a billion years; the outer edge comes from the observation that Mars *does* appear to have had liquid water on its surface some 3.9 b.y. ago.

Note that in these units the boundaries of the HZ lie at slightly higher stellar flux for hot, bright stars, and at lower flux for cool, dim stars. That is because the stellar radiation is blue-shifted (red-shifted) relative to our Sun, causing the planet's effective albedo to be higher (lower). Note also that Earth is near the inner edge of the HZ in this diagram, and that Mars is just inside the outer edge. A 10 percent increase in solar flux, which is expected to occur within the next 1 b.y., would be sufficient to push the inner HZ edge out past Earth, according to these calculations, possibly causing it to lose its oceans. Despite being within the HZ, Mars is not habitable (on its surface) because it is not able to recycle volatiles and because it has lost much of its atmosphere to space.

Implications: Our group has argued [11] that a conservative definition of the HZ should be used when designing direct-imaging telescopes like HabEx or LUVOIR. One wants to make sure that the telescopes are capable of finding Earth-like planets, if they exist. Once such a telescope is built and launched, however, we can afford to relax this assumption and look for planets that lie anywhere near this region. That said, interpretations of a planet's spectrum may continue to be influenced by its position relative to the HZ. Large amounts of O₂ for example, seen on a planet inside the HZ inner edge would likely be caused by photodissociation of H₂O, followed by escape of H to space, and not by photosynthesis. But there is no reason to think that we would overlook potentially habitable planets simply because we started from a conservative definition of the HZ. Rather, observers will almost certainly study every planet that they can see, and these observations will ultimately inform us as to whether other habitable planets exist.

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PLATE TECTONICS, HABITABILTY AND LIFE

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Introduction: The role of plate tectonics as a requirement for the habitability of terrestrial planets is being increasingly discussed [e.g., 1], in particular, in view of the growing number of confirmed exoplanets. A simple, most-used concept requires the thermodynamic stability of liquid water on the surface of a planet. Calculations for a model Earth lacking plate tectonics but degassing CO₂, N₂, and H₂O to form a surface ocean and a secondary atmosphere [2] suggest that liquid water (albeit only a few percent of an ocean mass) can be maintained on the surface for 4.5 Ga and beyond. For the more complex-featured habitability of Earth, the plate tectonics geochemical cycle is widely accepted to be fundamental [e.g., 3]. It maintains climate stability, keeps seawater volume and composition near equilibrium and causes the formation and persistence of continents where life can freely harvest solar energy through photosynthesis. Oxidization of an initially reduced Earth interior through plate tectonics is a possible mechanism for the increase of free oxygen in the atmosphere around 2.3 Ga b.p. [e.g., 4], a pre-requisite for more evolved eukaryotic life. The oxidization would diminish a sink in the oxygen budget of the atmosphere by lowering the rate of outgassing of chemically reduceing gases. Moreover, plate tectonics promotes increased heat transport through mixing of cold lithosphere with the deep interior and thereby supports core cooling and the long-term activity of the geodynamo.

Less well known is whether, how, and to what extent life may have an effect on the interior of the planet and the workings of the plate tectonics machinery. The way plate tectonics operates and possibly its very existence depend on the presence of volatiles [e.g., 5]. Water, above all, affects tectonic and mantle deformation through its effect on the rheology: its presence can significantly lower the strength of surface rock and the effective viscosity of mantle rock [6]. The fact that Venus presently lacks plate tectonics, despite its similarities with the Earth, has been ascribed to it being so dry [7]. In addition, water can reduce the solidus temperature of rock by up to several hundred degrees [e.g. 8], thus causing a wet mantle to undergo significantly more differentiation through partial melting than a dry one. Rheological weakening and increased melt production will favor mantle cooling, the former by increased subduction, the latter through heat removal from the mantle through partial melting. Water is transported to the mantle via subduction of sediments and hydrated crustal rock. The partial relase of water in subduction zones and the reduction of the melting temperature of sedimentary, crustal and mantle wedge rock is fundamental to the production of continental crust [e.g., 9]. Thus, if the biosphere had a significant influence on wheathering and the formation of sediments [e.g., 10] and in lowering the activation energy for metamorphic reactions [e.g., 11] that bind water, a direct link between life and the dynamics of the interior could be established.

Plate Tectonics as a System of Feedback Cycles and the Biosphere: Plate tectonics can be considered as a natural system maintained in disequilibrium by feedback cycles. But would the operation of these feedback cycles necessarily lead to the habitable environment of the present Earth, with about half of the surface covered with land and the other half with oceans? We consider a plate-tectonics model of the thermal evolution of the Earth along with the evolution of the continental coverage and the mantle water budget [see also 12, 13], focusing on the feedback cycles that govern the mantle water budget and continental crust growth.

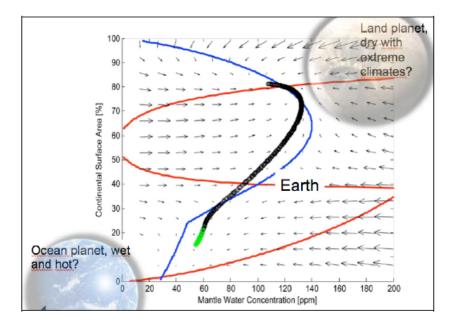
Feedback Cycles for Continental Growth and Mantle Water. The first couple of positive and negative feedback loops includes cycling of water into the mantle at subduction zones and outgassing at volcanic chains and mid-ocean ridges. Water will reduce the viscosity of mantle rock, and therefore increase the speed of mantle convection and plate subduction, eventually enhancing the rates of mantle water regassing. This positive feedback will be damped by the increased outgassing of the mantle through volcanism.

The second couple of feedback loops includes the production and erosion of continental crust. Continents grow by volcanism above subduction zones, whose total length is determined by the total area of the continents and whose increase will increase the growth rate. The erosion rate of the continents is proportional to the total continental surface area, too, which will tend to balance the positive effect of continental growth. The rate of sediment subduction affects the rate of transport of water to the mantle and the production rate of new continental crust.

Bistability. We show how the system starting with a single stable fixed point bifurcates as the planet cools to develop two stable and one unstable fixed point in a plane defined by the mantle water concentration and the surface area of continents (see figure below). The time of bifurcation depends on the strengths of the positive and negative feedbacks and thus on the effects of water on the rheology and melting points and on the



assumed wheathering rate. The two stable points represent 1) a planet (mostly) covered by continental crust with a wet mantle and 2) a planet (mostly) covered by oceans with a dry mantle. The unstable fixed point is close to the present Earth, in between the two stable extreme states.



We calculate evolutionary paths and find that the final state reached after 4.5Ga depends on the initial conditions of potential mantle temperature (1800-2200 K), initial mantle water content (0-200 ppm), and time of onset of plate tectonics (0-2 Ga), given rheological and other material parameters. Choosing random combinations of initial conditions, we find that the majority (about 75%) of model planets will be almost entirely covered by continental crust, while a secondary maximum (about 20%) exists for ocean planets. This should be an interesting datum to compare with exoplanet statistics.

Only a few percent of the models reach the present Earth state.

Impact of the Biosphere. By enhancing continental weathering and eventually the sediment transport into subduction zones, the biosphere impacts both pairs of feedback cycles. Model calculations with reduced wheathering rates – thus modeling an abiotic Earth – show the unstable fixed point to move towards larger values of continent coverage and the model planet to evolve towards the ocean planet fixed point. Continents first growing and then shrinking in time, contrary to what is observed for Earth. The Biosphere might, therefore, play a crucial role in regulating Earth's system and keep the continental crust coverage and mantle water budget at its present state.

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PLATE TECTONICS AND SURFACE HABITABILITY

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Introduction: One of the biggest puzzles when it comes to the origin and evolution of life, is the peculiar characteristics that our Earth has in contrast to the planets and moons of the solar system, and what (if) we can learn from that. Earth orbits the sun at the right distance to allow for liquid water at its surface since the Moon-forming impact, but it also posses elevated land coverage that life was thriving on. The oceanic crust is recycled into the mantle on geological time scales by plate tectonics. Volcanic activity leads to continuous feeding of greenhouse gases into the atmosphere, compensated by carbon sinks via weathering in the global carbon cycle. The surface of Earth is shielded from harmful radiation by a magnetic field. None of the other bodies in the solar system show all of these characteristics – and for none of them were we so far successful in finding traces of life. Are all these astro- and geophysical processes and properties necessary for a planet to be habitable for any kind of life? Are they related to each other? Do we need plate tectonics and active volcanism together with a magnetic field for life to develop into complex beings such as us?

The role of plate tectonics on Earth: The impact that plate tectonics had on the evolution of Earth and life at its surface seems to be immense - without the rise of the continents (and continental shelfs), it is questionable how effective the photosynthesis would have become, and the impact of life on the atmosphere may have been much less - depending on the biomass that can evolve without any larger land coverage or shallow water regions around continental areas. The great oxygenation event, which on Earth may be a result of multiple effects (invention of photosynthesis, inefficient geochemical buffering of oxygen at the surface due to changes in crustal composition [1], change in redox state of Earth's mantle reflecting a change in outgassing products [2], change of submarine volcanism to subaerial volcanism [3]), seems to be strongly coupled to the existence (and possibly initiation) of plate tectonics at that time. In addition, the cooling effect that subducting plates have on the mantle, leads to an increased heat flux at the core-mantle boundary, which has a positive impact on maintaining a magnetic dynamo. Regulation of the atmosphere depends on both continental weathering (via life-enhanced silicate-carbon cycle) and seafloor weathering – but the latter process may have been dominant during early Earth [4], and does not need active plate tectonics but instead only replenishing of fresh, basaltic crust at the surface, which could as well be delivered by volcanic activity from hotspots or super-plumes in the mantle. If plate tectonics would not have been active on Earth, it is difficult to imagine that life would have evolved in the same way as it did, and maybe macroscopic forms of life, as they appeared on Earth few hundreds of million years ago, would not have been possible without plate tectonics.

A habitable planet without plate tectonics? What if Mars would have accreted more material and would be twice as large, comparable to Earth. Would it be impossible to find habitable niches at its surface without plate tectonics? If Mars would be more massive, its atmosphere would be expected to be much denser possibly with a stronger greenhouse effect, since atmospheric loss would have been less efficient during its early evolution, and more volatiles could have accumulated due to an increased delivery of volatile-rich material during the later stage of accretion [5,6]. Volcanic activity might still persist after billions of years, and would be more active than on Mars due to the larger mass (and therefore higher amount of radioactive heat sources in the mantle) – comparable maybe more to Venus' activity. Surface water would then be possible, if the atmosphere would have the right composition of greenhouse gases over long timescales, compensated by seafloor weathering. However, in the scaled-up Mars scenzario, an Earth-like dynamo activity would not be expected. But life is inventive and may be able to overcome the missing shielding of the surface from harmful radiation – for example by living at or in the seafloor of the ocean. These arguments are purely speculative, but if Mars would be similar to Earth in size, it could be habitable over geological timescales even without plate tectonics, even though it is questionable how evolved life would have become under such circumstances.

However, the mass can also play a negative role for the evolution of the atmosphere and hence surface temperatures and potential surface habitability. For more massive super-Earths, plate tectonics may be therefore more important. If no substantial amounts of the primary atmosphere (from gas accretion and magma ocean outgassing stages [7]) survive, super-Earths may not be able to produce a dense-enough atmosphere to have liquid water at the surface, as long as they do not evolve into a plate-tectonics state [6]. For these planets, plate tectonics would be a necessary ingredient to build a dense-enough atmosphere for water to be liquid at the surface, and hence for (Earth-like) life to form and evolve.

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STAGNANT-LID TECTONICS DURING THE ARCHAEAN AND DELAYED ONSET OF PLATE TECTONICS

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Introduction: A major change in Earth's geodynamics occurred ~3 billion years (Gyr) ago [1, 2] that was followed by the great oxidation event ~2.4 Gyr ago [3]. However, it is not clear if those events can be related in terms of habitability. Solving one part of the puzzle is to understand what represents this change at ~3 Gyr. Since the Archean (between 4 to 2.5 Gyr ago) was much hotter than the present time because of higher rates of internal heat production, it is traditionally accepted that the mantle was convecting faster, but also that plates at the surface of the Earth were also moving faster. Short-lived isotope systems can help investigating the geological processes that oc-curred during the Archean because their production stopped at some point in the past. As such, the system 146Sm-142Nd where 146Sm was extinct ~0.5 Gyr after the formation of the solar system is par-ticularly useful to investigate the Earth's early geodynamics.

Results: By using this system, we found a resolvable positive anomaly of $\mu_{142}Nd = +7 \pm 3$ ppm in a 2.7 Gyr old tholeiitic lava flow from the Abitibi Greenstone Belt indicating that early mantle heterogeneities formed between 4 and 4.5 Gyr persisted ~1.8 Gyr after Earth's formation [4]. This result contradicts the expected rapid early (~0.1 Gyr) [5-7], as well as the slower recent (~1 Gyr) mixing rates in the convecting mantle [6-9]. We developed a numerical modelling [4, 10, 11] that suggests that inefficient convective mixing can occur even in a highly convective mantle in absence of plate tectonics, i.e. in a stagnant-lid regime. Our model allows only sporadic and short subduction episodes throughout the Hadean and Archean in order to explain the long-term preservation of chemical anomalies in a highly convective mantle.

Conclusion: The combination of the geochemical signal and the numerical modelling suggests that the major change that occurred ~3 Gyr ago is likely related to the transition between stagnant-lid regime to modern style plate tectonics, i.e. mobile-lid regime. The inefficient mantle mixing in the early Earth's convective mantle due to stagnant-lid tectonics is likely to be similar to these mechanisms operating in other terrestrial planets such as Mars. The onset of modern plate tectonics had major implications for the evolution of the Earth [12]. First, effects on the climate as major Neoproterozoic glaciations have been related to continental breakups and an associated increase in explosive volcanism, logical consequences of subduction plate tectonics [12, 13]. Second, triggering of true polar wander may be related to global changes in mantle convection and plate motions, the most important reason being continuous injection of cold slabs within the mantle though subduction processes [14]. Third, effects on the biosphere may have been important as biological activity may have been enhanced due to continuous volcanism and orogeny that provided more nutrients, possibly having a link with the great oxygenation event [15].

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IMPLICATIONS OF A NON-PLATE TECTONIC MODEL FOR THE ARCHAEAN EARTH

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Archaean litho-tectonic associations are very different from Phanerozoic ones, and there are fundamental geochemical differences between modern arc magmas and Archaean calc-alkaline suites that imply modern type subduction was not active then. Thermo-mechanical modeling implies that oceanic lithosphere lacked a stable lithospheric mantle layer in Archaean time because of vigorous unsteady induced thermal convection, making Archaean oceanic crust unsubductable. These observations falsify the hypothesis that modern-style Plate Tectonics and active subduction were active on Earth prior to 2.5 Ga. It is proposed instead that the Hadean-Archaean Earth was in unstable stagnant-lid mode until ~2.5 Ga. This hypothesis resolves many paradoxical aspects of Archaean geology, magma-genesis and mantle geochemical and isotopic evolution. Stagnant-lid planets are inefficient at evacuating heat and numerical models predict periodic mantle overturns. Model results and Archaean age patterns suggest that overturns lasted ~100 my and were separated by stagnant-lid episodes lasting ~300-400 my. During overturns, upwelling zones would have supplied abundant basalt and komatiite, resurfacing and reworking much of the existing crust, creating prominent planet-wide magmatic age peaks, and probably kick-starting continent genesis. Syn-overturn mantle flow drove continental drift, creating soft accretionary/subcretionary orogens. This model is validated by comparisons with Venus, which preserves evidence for continental drift on a planet without Plate Tectonics; and the NE Superior craton, where age and Nd isotopic data imply most Neo-Archaean granitoids are reworked older felsic plutons, with <50% of older domains surviving this overturn event intact. Extrapolating this survival rate into the past implies repeated large-scale remelting of existing crust during overturns, and consequent high magmatic fluxes which would have had a negative impact on complex biota, which may partly explain the slow rate of evolution on the early Earth. With time, the decrease in radiogenic heat allowed Earth's oceanic lithosphere to stiffen and densify, making subduction and Plate Tectonics possible. The presence of a hydrosphere is needed to cool the oceanic lithosphere enough for this to occur.



COSMIC RAYS-INDUCED FORMATION OF SUPER-COMPLEX AMINO ACID PRECURSORS IN SPACE

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Introduction: Since a wide variety of organics has been detected in extraterrestrial bodies like carbonaceous chondrites [1], extraterrestrial organics are probable sources for the first terrestrial life. Amino acids in carbonaceous chondrites increased after acid-hydrolysis. Laboratory experiments simulating extraterrestrial environments showed that not free amino acids but amino acid precursors were abiotically formed [2,3]. It has not been proved, however, what kinds of amino acid precursors were formed in space and delivered to the Earth. Extraterrestrial organics are exposed to cosmic rays, high-energy photons (including gamma rays [4]) before delivered to the Earth. It is thus important to examine stability of amino acid precursors in space. We experimentally investigated possible formation of amino acid precursors against heavy ions, gamma rays, UV and soft X-rays.

Prebiotic Syntheses of Amino Acid Precursors: Frozen (77 K) mixtures of methanol, ammonia and water with various mixing ratios were irradiated with high-energy carbon ions (290 MeV/u) from HIMAC, NIRS, Japan. Gaseous mixtures of carbon monoxide, ammonia and water were irradiated with high-energy protons (2.5 MeV) from a Tandem accelerator, Tokyo Tech, Japan. Amino acids were detected in all the irradiation products only after acid-hydrolysis, even when a 10:1:111 (molar ratio) mixture of methanol, ammonia and water was irradiated. Thus it is plausible that amino acid precursors could be formed in ice mantles of interstellar dust particles. Their FT-IR and XANES spectra suggested that the irradiation products had super-complex structures with amide bond moieties, rather than nitrile moieties. Fractionation studies showed that simple well-known precursors such as aminonitriles and hydantoins were not major ones.

Stability Against radiation: Aminoacetonitrile (AAN) and hydantoin (Hyd) were candidate precursors of glycine (Gly). We examined stability of Gly, AAN, Hyd and CAW (the product synthesized by proton irradiation of carbon monoxide, ammonia and water): Carbon ions (290 MeV/u) were irradiated from HIMAC, NIRS to frozen solution of the compounds to evaluate stability in molecular clouds. Gamma rays from a ⁶⁰Co source, Tokyo Tech, were irradiated to aqueous solution of the compounds to simulate reactions in meteorite parent bodies. In these experiments, CAW showed the highest recovery: Gly yield was the lowest.

Conclusion: It is plausible that *amino acid precursors* could be formed in ice mantles of interstellar dust particles by the action of cosmic rays. The structures of the precursors were unknown, but it was suggested that they were not simple precursors but had super-complex structures. Such supercomplex amino acid precursors were much more stable than simple precursors and free amino acids in simulated space conditions. Thus we concluded complex amino acid precursors formed in space could be safely delivered to the primitive Earth, while free amino acids were not stable during delivery even if they were formed in space.

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ATTEMPTING TO CONSTRAIN A GEOLOGICAL AND CHEMICAL SCENARIO FOR THE ORIGIN OF LIFE

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Introduction: When considering life's aetiology there are many problems that must be confronted, the most fundamental being the prebiotic synthesis of the minimum set of molecules which could give rise to life. Irrevocably linked to this problem, is the question of the physical place on Earth that the synthesis occurred, as the surrounding environment would have a direct bearing on the types of chemistry which were feasible¹. For example, if deep sea vents are chosen as the location to investigate for the origin of life, photochemical reactions must be ruled out. This raises a question in itself – does one first consider a geochemical environment which one imagines could kick-start life and then (ideally) explore the chemistry which is possible within these bounds, or does one investigate a synthesis which one hopes to be prebiotically plausible and then try and fit that synthesis to an early Earth geological setting? The literature suggests that taking an inflexible stance on 'geology first' or 'chemistry first' is counterproductive to progression, and consequently we have tried to adopt an intermediary approach.

By considering a potentially prebiotic, geological source of phosphate, necessary for the prebiotic synthesis of activated nucleotides², new chemistry was uncovered which led to the discovery of a protometabolic network^{3,4,5}. Concurrently, a geochemical scenario unfolded which is suggestive of flow and semi-batch chemistry, and by bootstrapping between chemistry and geology, more reagents, reactions and (proto) biomolecules were found⁵. Attempting to recapitulate this fluvial model using flow chemistry techniques, we have discovered further novel aspects of prebiotic chemistry which enhance the plausibility of the synthetic route and fit with the geochemical model⁶.

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PROBING LIFE'S ORIGINS THROUGH BIOLOGICAL REDUCTION

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Biology's theoretical development over much of the 20th century has been built on the conviction that biology is not reducible to physics and chemistry, that life's whole is more than the sum of its parts [1]. Interestingly, the spectacular advances in molecular biology during the last half century merely served to reinforce that view. Despite the detailed molecular information that was forthcoming, the molecular approach offered few insights into life's unique emergent properties and limited information on life's origins. As a consequence, biology's conceptual base has remained biological, and its central concepts to this day continue to be expressed in biological terms - natural selection, fitness, mutation, species, genes, etc. In this talk I will argue that if life is considered as 'process' rather than as 'things' [2], then reduction (of the process, not the things) does appear feasible, and may be able to offer insights into life's physical origins, as well as the basis for its holistic properties, notably agency, function, cognition.

The analysis is based on the insight that the entire evolutionary pathway, from chemical beginnings through to complex life, can be considered as one single continuous process. Its directive is the drive toward greater stability, but an alternative stability kind to traditional thermodynamic stability, one we have termed *dynamic kinetically stability* (DKS) [3]. That stability kind is based on *persistence* rather than *energy*. Furthermore, we have proposed that the primary chemical step which initiated that evolutionary process was the excitation of a replicative chemical system into the DKS state. Without that activation step, which could be considered a phase transition, the evolutionary process – complexification toward extant life – would not have been possible. It is within that primordial DKS system, that life's rudimentary holistic character, as well as its earliest organizational character, can be identified – dynamic, non-equilibrium, energy-fueled.

More generally, if successful epistemological reduction of biology to physics and chemistry could be demonstrated, it would be a step toward the creation of a unified material framework encompassing both physical and biological worlds, as opposed to the largely disparate physical and biological conceptual worlds that exist today.

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MESSY CHEMISTRY: STRUCTURE AND FUNCTIONALITY OF HYPERBRANCHED POLYESTERS

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Introduction: The classical approach towards the origins of life usually concentrates on studies of isolated reactions and pure chemical synthesis systems. However, it has been long noted that chemistry in prebiotically plausible scenarios generate intractable heterogeneous mixtures of compounds. The appearance of tarry polymers was recorded in the Miller-Urey experiment[1], subsequently studied hydrogen cyanide (HCN) polymers [2,3] and formaldehyde condensation [4,5]. We are interested in a new approach to the origin of life, so-called "messy chemistry" that studies the properties of these complex mixtures that give rise to life-like systems. Messy chemistry hypothesizes that life started with complex reaction networks that are common to prebiotic chemistry, evolved as a complex reaction network into biochemistry that constitutes a complex reaction network. Aspects of the messy chemistry research involve the study of the functionality of prebiotically plausible messy polymers, development of better analytical methods suitable for messy chemistries, including functional measurements experimental and theoretical modeling of the processes occurring in complex chemical systems. The ultimate goal of the "messy chemistry" is to understand the transition between messy, marginally controlled, prebiotic systems into well-orchestrated life-like chemical networks, or the origin of life. Herein we present several aspects of our studies into the synthesis and function of hyberbranched polyesters (HBPE).

Potential HBPE role in chemical evolution: The topology of HBPE enforces globular structure and allows for a controlled microenvironment surrounding the core similar to globular protein structures present in enzymes. To test this hypothesis we have studied two systems. First system is a proof-of-principle study of amine-bearing HBPE catalysts [6]. Our results showed that tertiary amine-bearing hyperbranched polyesters to form hydrophobic pockets as a reaction-promoting medium for the Kemp elimination reaction. The second system is probing the ability of HBPE to support metal-sulfide particles that catalyze prebiotically and biologically relevant redox reactions.

Selective synthesis of HBPE under wetting-drying cycles: HBPEs can be synthesized by subjecting multifunctional organic acids and alcohol mixtures to mild heating under solventless conditions [7]. This method, however, produces a multitude of polymeric products varied in size and shape. Synthesis of HBPE under wetting-drying cycles can provide the means of selection for specific products based on their function and structure. Period of heating the open vessel promotes esterification. Even though periodic sample rehydration promotes hydrolysis, successive iterations of wetting- drying cycles result in polymer yields and molecular weight distributions in excess of that observed after a heating alone. Products less prone to hydrolysis would tend to persist in the system at the expense of the rest. The hydrolysis patterns of HBPEs differs from linear polymer ones. The globular nature of HBPEs prevents or delays the water intrusion into the core, slowing down the hydrolysis process and resulting in macromolecular surface erosion rather than breakdown. When day-night cycling applied to HPBE condensation, the first drying phase will result in a mixture of linear, branched and mixed polymers. During the hydrated phases linear portions of the polymer would be more susceptible to hydrolysis than their branched counterparts, therefore it is reasonable to assume that after a number of cycles the makeup of the polymer would consist of predominantly branched arcitechtures. We will present size-exclusion chromatography and NMR data in support of the above assumption.

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CO-EVOLUTION OF METABOLISM AND CELLULAR COMPARTMENTS

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Introduction: Contemporary biology relies on two types of functional polymers - nucleic acids and proteins – encapsulated in membrane-bound compartments. Nucleic acids are primarily involved in expressing and transferring genetic information, whereas proteins mediate most other cellular functions, in particular, chemical catalysis. It has been long assumed that only one of these polymers existed at the origin of life and participated in both information transfer and catalysis. According to the canonical RNA World hypothesis, this polymer was RNA. Proteins emerged later, catalyzed by ribozymes. According to the alternative, Metabolism First hypothesis, basic reactions of life were initially aided by inorganic surfaces, small organic molecules and, eventually, randomly synthesized small proteins. However, despite extensive efforts, considerable difficulties persist in gathering support for either of these hypotheses. In view of these difficulties, it is justified to explore a possibility that metabolism, information polymers, cellular compartments and energy transduction systems supporting living entities co-evolved from the earliest stages of the origin of life.

Co-evolution of Metabolism and Membranes: Protocellular boundaries were inextricably connected to the metabolism they encapsulated: to be inheritable, early metabolism must have led to an increased rate of growth and division of vesicles and, similarly, transport through vesicle boundaries must have supported the evolution of metabolism. Permeation through vesicle walls would have been a robust mechanism to do so, although other mechanisms, such as disruption and subsequent reformation of vesicles were also possible. Everything that could not have been delivered from the environment had to be produced and retained inside protocells. In other words, evolution of metabolism influenced membranes, and evolution of membranes influenced metabolism. General mechanisms and specific examples of such coupling will be discussed.

An example of the influence of metabolism on membranes is a process whereby a dipeptide trapped inside fatty-acid vesicles catalyzes the formation of another dipeptide that interacts with vesicle membranes and, by doing so, promotes their growth through fusion with micelles. It has been shown in computer simulations that the latter dipeptide has to be nonpolar to form fusion-inducing hydrophobic patches at the surface of vesicles. This principle is general and applies not only to dipeptides but also to other hydrophobic molecules (see Fig. 1).

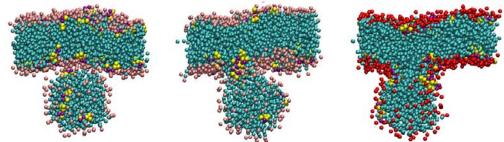


Fig. 1 Hydrophobic dipeptides (yellow) mediate vesicle growth and division through their fusion with micelles.

Co-evolution of Metabolism and Membrane Proteins. It is hypothesized that he earliest membrane walls were built of fatty acids. The appearance of phospholipids imparted selective advantage to protocells bound by phospholipid-containing membranes, eventually driving fatty-acid vesicles to extinction. Phospholipid membranes, however, are nearly impermeable to charged species. Yet, the ability to transport ions across membranes was vital for regulating cellular volume, pH homeostasis, generating energy and sensing the environment. For this reason, life evolved ion channels, protein structures surrounding water-filled pores in the membrane that facilitate ion transport. A scenario for this evolutionary process has been developed.

Membranes and Bioenergetics. One of the most important events in the origin and early evolution of life was the emergence of an energy transduction system based on electrochemical gradient across membranes. This allowed the nascent living systems to reliably harvest environmental energy instead of relying of fickle supply of high energy chemicals in the surrounding medium. Electrochemical energy transduction systems consist of two main steps. Proton pumps use external energy, for example light, to generate proton gradient across a membrane. This gradient is subsequently used to drive synthesis of the high-energy compound, adenosine triphosphate, the common energy currency of life. Taken together, energy transduction is carried out by a complex, multicomponent system. So far, no convincing clues to the evolutionary origins of this system have been uncovered. Instead of tracing these origins we propose to demonstrate that a simple, biological system can be capable of energy transduction.



TRANSITION FROM LOW FIDELITY GENE EXPRESSION TO HIGH FIDELITY

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Each life has and transfers its information from origins of life. As well as nucleotide sequence, concentrations of molecules can be crucial information for life. Because of importance of those lines of information, comparison between "metabolism first" and "replication first" attract researchers in this field. From fidelity point view, polynucleotide has strong points in correct transfer of information because of base complementarity in replication. However, life must have emerged from low fidelity polymerization system, considering that present systems have evolved mechanisms to achieve high fidelity. Thus we need to explore properties of primitive life with lower fidelity than that of present life. Similar question in fidelity by modification of cell-free translation, by using tRNA variant with anticodon replacement [1-2]. As well as moderate error rate in other steps for gene expression and replication, the low fidelity of the code could accelerate evolution of polymer sequence. On contrary, gene expression and replication with error prevents fine tune in evolution. In other words, trade-off of those aspects in gene expression defines transitions of life from low fidelity system to high fidelity one. Similar trade-off would be important in comparison between "metabolism first" and "replication first".

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THE RNA WORLD: SELF-REPLICATING AND EVOLVING SYSTEMS OF CATALYTIC RNAS U. F. Muller¹. ¹Department of Chemistry and Biochemistry, University of California, San Diego; La Jolla, California, USA. ufmuller@ucsd.edu

Introduction: To explain how life may have arisen from an abiotic world the RNA world hypothesis was developed in the 1960s [1-4] and experienced increased interest after the first catalytic RNAs were discovered in the 1980s [5-7]. The requirement for this hypothesis came from the conundrum that in today's life forms DNA is dependent on proteins for its replication, and proteins depend on DNA for their information. It would have been astronomically unlikely for such an interdependent system to directly originate from a prebiotic environment. The solution was that RNA could fulfill both roles in one molecule: The RNA world hypothesis states that there was a stage in the early evolution of life in which RNA acted as genome and as the only genome-encoded catalyst.

Over the last 4 decades evidence has accumulated that there was indeed an early stage in the evolution of life in which RNA was the central macromolecule. The ribosome - which is responsible for all encoded protein synthesis - is a catalytic RNA [8, 9] as well as RNase P [7], nucleotides are the building blocks for most cofactors although there would be no chemical necessity for them [10], and DNA monomers are synthesized from RNA monomers [11]. Importantly, in vitro selection experiments have shown that RNAs would be able to catalyze all reactions that would be required for a self-replicating RNA system [12, 13].

Lab studies on the RNA world: Wet-lab model systems of self-replicating nucleic acids have been generated [14-17] and some of their emerging phenomena been studied [18]. However, systems that achieve self-replication use RNA fragments as substrates, which limits their evolvability. In contrast, a model system that uses nucleotide monomers as substrates [19] has generated a small catalytic RNA [20] but not yet achieved self-replication. Two major goals of this line of research are to (i) achieve a self-replicating and evolving system based on nucleotide monomers, and (ii) to identify pathways how such a system could have bootstrapped itself out of a prebiotic environment.

(i) To address how RNA could have self replicated, several efforts are focused on exploring different cofactors [21-23]. Importantly, there may never have been a pure RNA world, and DNA may have been there from the beginning [24]. Additionally, the exploration of phosphate activation groups has shown that activated phosphates may have been continuously involved in the origin of life, from prebiotic chemistry to modern biology's nucleoside triphosphates [25-28]. My own research has focused recently on the question whether, and how the prebiotically plausible compound trimetaphosphate [29, 30] could have been used as energy source for RNA world organisms [26, 31].

(ii) To address how an RNA world could have emerged from a prebiotically plausible environment there is growing interest in model systems that are chemically more complex, involve less or no purification steps, and show less linear / more network-like prebiotic chemical pathways [32-34]. Another idea is that a different polymer such as TNA (Threose Nucleic Acid) may have preceded RNA [35]. While TNA is easier to synthesize in a prebiotic environment this idea creates the problem how information from the TNA world would have been transferred into the RNA world stage.

'Genome first' and 'metabolism first' hypotheses: The debate of 'genome first' versus 'metabolism first' is unnecessary because the answer depends on the definition of terms. If the definition of a living system is 'a molecular system that is able to self-replicate and undergo open-ended Darwinian evolution' then 'life' comes into existence in the instance when a genome has replicated and evolved. The definition of metabolism as 'the chemical processes that occur within a living system' means that the same chemical processes that occured in the environment before the existence of life turn into metabolic processes as soon as they are used by a living system. Together, these definitions would mean that 'genome' and 'metabolism' would originate in the same instant, by definition.

A useful example is the finding of the same compounds in meteorites as well as constituents of the citric acid cycle [36]. This does not mean that living organisms generated these compounds in the



meteorites. Instead, it means that some chemical pathways occur under a wide range of conditions in the universe. As soon as they can be utilized (and often catalyzed to be most useful) by a living organism [37] they are defined as metabolism.

The chemical processes required for the first RNA polymers must have provided the raw material that allowed the early RNA world to replicate. While major advances have been made in how nucleotides could have been generated [38, 39] it is an open question whether RNA polymers of a sufficient complexity to catalyze self-replication could have been generated directly from a prebiotic environment. A pre-RNA world such as TNA may be necessary to have jump-started the earliest life from a prebiotic soup.

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REPRODUCTION OF A SET OF DIVERSE MOLECULES, MINORITY CONTROL, AND ARRIVAL OF EVOLVABILITY

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How reproduction of 'protocells' with diverse chemical components has been achieved from just a set of catalytic reactions, and how bioinformation has emerged from it to allow for evolvability are two basic questions in order to understand the origin of life. I will discuss some basic theoretical issues to address the questions.

- (1) Diversity: In general, a protocell with fewer components can grow faster. In spite of this pressure to simplification, there are generally diverse components within a cell. Transition to diversity due to resource limitation is discussed.
- (2) Kinetic origin of information and relevance of minority component: Among diverse components of mutually catalytic reaction, we show that a minority component needed for reproduction plays the role of genetic carrier and allows for the exponential growth.
- (3) Reproduction of a compartment: In a reaction-diffusion system of mutually catalytic reproduction, formation of a compartment of an ensemble of molecules and its division is achieved with the aid of the replication of minority molecule. This allows for a growth-division cycle of protocells.
- (4) Symmetry breaking between function and information in a system with multilevel reproduction: In a protocell system with mutually catalytic molecules, each molecule tends to lose its catalytic activity in order to increase its replication rate, whereas the growth rate of the protocell is decreased by it. This antagonistic drive will lead to the separation of roles in molecules and allowing for the origin of bioinformation..

This study is in collaboration with Atsushi Kamimura (1-3), and Nobuto Takeuchi(4).

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EVOLUTION OF LIFE REVEALED FROM GENETIC INFORMATION

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Introduction: All of the living species on Earth have been evolved from the organism called LUCA (Last Universal Common Ancestor), senancestor or Commonote [1]. We defined the Commonote as the last and the latest common ancestral species, which shared the gene pool.

We have analyzed the genes of the translation system. Because the system is essential and possessed by all species, it is ideal to analyze the evolution of species. From the analysis of the genes of the translation system following points were revealed [2]. 1) Commonote was split into two groups: Bacteria and Archaea + Eucarya. 2) Archae and Eucarya were not clearly separated one another and the later was included in the former.

We have also inferred and reproduced ancestral protein, NDK (nucleoside di-phosphate kinase), possessed by the common ancestors of Bacteria and Archaea, and by Commonote. Analysis of the reproduced ancient NDKs showed extremely high thermal stability. The thermal stability of NDK has high correlation index to the growth temperature of the species. Accordingly, the common ancestors of Bacteria and Archaea, and Commonote were inferred to be the species once lived in very high temperature environment [3, 4].

It is also possible to obtain the information on the environmental temperature by analyzing the resserected proteins of land plant and marin cyanobacteria [5, 6].

The combination of the analysis of genetic information and genetic engineering technology is a powerful tool to elucidate the characteristics of the ancestral life forms. Our results suggest that the Commonote was living in very hot environment.

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DID EMERGED LANDS CONTROL THE LIFE ORIGIN AND DEVELOPMENT?

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Since the early 2000s several authors proposed scenarios for emergence of life that requires the alternation of dry and aqueous phases (Commeyras *et al.*, 2002; Lathe, 2004; Deamer, 2017), which necessitates that part of the continental crust was above the sea level. On the other hand, nutrients, such as phosphorus, necessary to sustain and develop life, are provided to the ocean by continent weathering through river discharges. Here too, emerged lands are required.

However, some computed models, mainly based on isostatic considerations, lead to the conclusion that until the end of Archaean times almost the whole planet was covered by water (Vlaar, 2000; Flament *et al.*, 2008); significant amounts of land emerging only from about 2.5 Ga. In the same time, geochemical approaches, based on Sr isotopes (Dhuime *et al.*, 2015) or on Ti isotopes (Greber *et al.*, 2017) concluded that continental lands were emerged since at least 3.5-3.8 Ga or even before.

On another hand, sedimentary investigations performed for instance on 3.2 Ga-old sandstones from Barberton greenstone belt in South Africa, demonstrated that at this time, the anomalistic month was close to 20 days while, today, it is of 27.55 days (Eriksson and Simpson, 2000). This is accounted by the fact that at that time the Earth-moon distance was ~200 000 km when it is 384 400 km today. Consequently, tidal forces were greater than today, such that it has been proposed that intertidal zone could have extended several 100 km inland (Lathe, 2004). Even, if Archaean tides were not so drastically strong, they were stronger than today, which would have two important effects : i) they would have subjected coastal zones to fast alternation of flooding and drying episodes; ii) they would have had significant erosive power, making the transfer of nutrients from land to the ocean more efficient.

In summary, it appears that the existence of emerged land before 2.5 Ga, is a key but also highly controversial question. Indeed, the absence of emerged land precludes any efficient supply of nutrients (eg. phosphorus) to the ocean. The only remaining source of energy and nutrients would have been the hydrothermal systems, in which case, life would have been confined to the bottom of oceans during almost the whole first half of Earth history

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PRIMITIVE MEMBRANES: COMPOSITION AND ENVIRONMENTAL IMPACT

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Compartmentalization plays an central role in the definition of cellular life, both in terms of shaping/preserving the identity of the cell and supporting essential metabolic functions, such as signaling and biosensing, and energy harvesting [1]. The intricate nature of the molecular interactions that characterize the cellular machinery hints at a co-evolution of the compartment and the other molecular species involved. The importance of a compartmentalization early on in the development of cellular life or its chemical precursors seems to be undisputable. However, the nature of its chemical embodiment (type of chemicals involved, morphology), which was influenced by the chemical inventory on early Earth and the geochemical environment, remains highly debated due to the lack of direct evidence [2].

We will here review the research on compartmentalization systems, emphasizing amphiphile based ones. In particular, we will show that a large number of such chemicals are prebiotically plausible, that, in constrast with common wisdom, their assembly into structures that could serve as compartment for chemical reactions, can occur under extreme environmental conditions (pH, ionic strength, and temperature)[3], and finally that the formation of compartment can be supported by non-amphiphilic molecules that could have been the precursors of other modern essential biomolecules[4]. This short survey will also highlight the importance of two concepts: chemical contiguity and chemical systems [5].

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PRE-GOE CHEMICAL OCEANOGRAPHY

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A late rise of large expanses of continents above sea level is strongly supported by the divergence of marine ⁸⁷Sr/⁸⁶Sr from the contemporaneous mantle values at the time of Great Oxygenation Event and by a large change of Zn isotope regime in banded iron formations. Subaerial continental expanses are important controls of ocean and atmosphere chemistry and the emergence and evolution of life. Weak erosion should be correlated with weak alkalinity fluxes to the ocean, no limestone deposition, weak phosphate fluxes and surface biological productivity, and rapidly fluctuating pH. Although some rare sedimentary sequences exist that look like their modern equivalents, like those of Barberton South Africa, most pre-GOE sedimentary sequences should be dominated by slowly deposited hypo- or anoxic abyssal sediments and long-term ocean chemistry controlled by hydrothermal inputs. The place for life before the GOE must have been very narrowly restricted. It is largely accepted that pre-GOE oceans were iron-rich and that Fe played the role played by modern Ca. We argue somewhere else (Thibon et al., submitted) that Banded Iron Formations are not necessarily associated with biological activity and that there is instead a strong connection between large volcanic eruptions and BIF forming events. I will attempt to provide an account of pre-GOE chemical oceanography, compare it with that of more recent oceans, and discuss the implications for the origin and evolution of life.



BIOLOGICAL COMPLEXITY, ORIGIN AND NATURE OF LIFE, AND MAJOR EVOLUTIONARY TRANSITIONS

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Biological systems reach hierarchical complexity that has no counterpart outside the realm of biology. The physical foundation for understanding the origin and evolution of complexity can be sought at the interface between the theory of frustrated states resulting in pattern formation in glass-like media and the theory of self-organized criticality (SOC). On the one hand, SOC has been shown to emerge in spin glass systems of high dimensionality. On the other hand, SOC is often viewed as the most appropriate physical description of evolutionary transitions in biology. I attempt to unify these two faces of SOC by showing that emergence of complex features in biological evolution typically if not always is triggered by frustration that is caused by competing interactions at different organizational levels. Competing interactions and frustrated states permeate biology at all organizational levels and are tightly linked to the ubiquitous competition for limiting resources. This perspective extends from the simple phenomena occurring in stripe glasses to large-scale events of biological evolution, such as major evolutionary transitions. One of the key types of conflict driving the evolution of biological complexity involves host-parasite interactions that are ubiquitous in biology and involve both arms race and cooperation. I will present thermodynamic-information theoretical argument that emergence of parasites is an inalienable feature of replicator systems and that such systems cannot be stable without evolving increasing complexity. These features are expected to be universal among all phenomena that can be meaningfully identified as "life".



QUEST FOR ANCESTORS OF EUKARYOTIC CELLS; IMPLICATIONS FROM EVOLUTION OF AMINOACYL TRNA SYNTHETASES.

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Extant cellular organisms are classified into two groups with different cell architectures, prokaryotes and eukaryotes. Prokaryotes have no apparent structures in which chromosome(s) are stored. Prokaryotes are also classified into distinct groups, Bacteria (Eubacteria) and Archaea (Archaebacteria) [1,2]. In contrast, Eukaryotes have a nucleus containing chromosomes (genome), a complex membrane system including endoplasmic reticulum and Golgi apparatus, and double-membrane organelles, such as mitochondrion and plastid (chloroplast). Origin of complex cellular structure of eukaryotes has been one of foci of studies on the early evolution of terrestrial life [3]. In particular, the origin of double-membrane organelles, mitochondrion and plastid with their own genomes and genetic system (replication, transcription, and translation), have been interested and explained by the hypotheses such as serial endosymbiosis [4].

Recent innovations in metagenome data and cultivation of bacteria and archaea provided information on uncultivated Bacterial and Archaeal genomes [5,6]. It potentially improves understanding of the phylogenetic relationships among the three domains. In Archaea, TACK superphylum consisting of Crenarchaeota, Thaum, Aigarchaeota, and Korarchaeota, [7], DPANN superphylum consisting of ultra-small cellular archaea (Diapherotrites and Parvarchaeota, Aenigmarchaeota, Nanoarchaeota, Nanohaloarchaeota, and Micrarchaeota) [5], and Asgard group (superphylum), consisting of Lokiarchaeota, Thorarchaeota, Odinarchaeota, and Heimdallarchaeota [8] have been proposed. The firstly recognized member of Asgard group, Lokiarchaeota, was reported as the member of TACK superphylum [9].

Based on the molecular phylogenetic analysis using small subunit ribosomal RNAs (SSU rRNAs), Woese proposed Bacteria, Archaea, and Eucarya as separate monophyletic groups and close relationship between Archaea and Eucarya [1,2]. This three-domain hypothesis has been supported by various molecular phylogenetic and phylogenomic studies [5,10,11].

On the other hand, two-domain hypothesis has been also proposed. The hypothesis implies that the eukaryotic ancestor was derived from a certain archaeal lineage. Crenarchaeota, TACK superphylum, Lokiarchaeota, and Asgard group have been proposed as the close relative of Eucarya [7-9,12,13]. The genomes of Asgard archaea were reported to carry the signature proteins of Eukarya related to cytoskeleton, membrane remodeling, and phagocytosis, suggesting that it is an ancestor of Eukarya [8].

Large-scale single-gene phylogenetic analyses using more recent data showed that Eukaryal genes were nested with either TACK superphylum or Euryarchaeota depending on the genes, which hide the true archaeal ancestor of Eukarya [14,15]. These analyses also suggested that many eukaryal genes were nested with several bacterial species, which show that lateral gene transfers from several bacteria lineages contributed to the formation of the last eukaryal common ancestor (LECA) [14-15].

Aminoacyl-tRNA synthetases (ARSs) are essential enzymes for translation in all extant organisms. ARSs have been used to resolve early evolution of life because of their universality and sequence conservation [17]. Since all known organisms use 20 standard amino acids in translation, the last universal common ancestor (LUCA, or Commonote) is thought to have used the same 20 standard amino acids in translation. There is also the possibility that the diversification of ARSs of each class occurred before the age of last universal common ancestor of all extant organisms [18]. Despite the complex evolutionary history, ARS is one of the best genes for the phylogenetic analysis of all extant organisms since the DNA sequences have been well conserved among all domains of life. Therefore, some ARSs were used as core genes for phylogenetic analyses to clarify the relationship between the proposed three domains of life [18,19]. Previous phylogenetic analyses of ARSs supported the three-



domain hypothesis [17,19,20]. However, for example, no sequences from TACK superphylum were used in the phylogenetic study by Brindefalk et al. [20]. Thus, it is important to conduct a molecular phylogenetic analysis of ARSs that includes new archaeal species and innovative technology to test the three-domain and the two-domain hypotheses.

When we constructed 23 ARS trees, none of them supported the three-domain hypothesis [21]. In 8 ARS trees, eukaryotic cytoplasmic ARSs are suggested to have archaeal origin. However, the archaeal close relatives of eukaryotic cytoplasmic ARSs are different among different archaeal groups, depending on the ARS. 4 eukaryotic cytoplasmic ARSs are also suggested to have bacterial origin, although the bacterial close relatives to the eukaryotic cytoplasmic ARSs are classified into two or three groups with distinct archaeal/bacterial origins. These suggest that the eukaryotic translation system is quite chimeric.

Based on our phylogenetic analyses of ARSs, we proposed a scenario on the process of eukaryogenesis. In this proposal, although we accept the concept that Eukarya has an origin closely related to the Asgard archaeal group, there had been numerical acquisitions of genes from various archaeal and bacterial groups via lateral gene transfer processes such as endosymbiosis and viral infection. In addition, we also proposed a classification where Eukaryotes and Archaebacteria (Archaea in Woese's classification [1,2]) are subdomains of domain Archaea [21].

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FROM LUCA TO LECA: HOW CONCEPTS OF THE LAST UNIVERSAL COMMON ANCESTOR MAY INFORM CONCEPTS OF THE LAST EUKARYOTIC COMMON ANCESTOR

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Understanding the nature of the Last Eukaryotic Common Ancestor (LECA) provides a framework in which to infer how eukaryotes originated and evolved. There is currently a large body of research attempting to gain insight into LECA using comparative genomic and phylogenetic methods. By definition, LECA is the biological state that gave rise to all extant eukaryotes. LECA is more, however, than a post-hoc label for any particular ancestral reconstruction. As well as being a broad reference point in a hypothesized historical space, LECA refers to underlying concepts of what the last common eukaryote ancestor was like, and what it could do. My talk (based on work with Michelle Leger, Jeremy Wideman, and Iñaki Ruiz-Trillo) will examine a continuum of different LECA conceptions and their implications for evolutionary reconstructions of early eukaryotes. This continuum runs from notions of LECA as a single cell, to LECA as an evolving population or species, and even further to LECA as a community. My focus will be a pangenomic notion of LECA, in which a diverse population exhibits genomic and phenotypic differences, despite being the same 'species'. I will compare this view of LECA with a more established multilineage view of LUCA, the Last Universal Common Ancestor at the origin of cellular life. This comparison may inform how we conceptualize key nodes in the evolution of living systems on Earth.



SOLAR SYSTEM FORMATION IN THE CONTEXT OF EXTRA-SOLAR PLANETS

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Introduction: Until the mid-1990s the Solar System was the prototype planetary system. Its radially-segregated architecture -- with small rocky planets close to the Sun and giant planets farther out -- was assumed to be the norm. We now know that this is not the case. The demographics of exoplanets show that the Solar System lies on a narrow branch of rare (~1% or less) outcomes of planet formation. In contrast, roughly half of all stars host close-in `super-Earths' or 'sub-Neptunes' and a significant fraction host giant planets on orbits very different than Jupiter's.

Exoplanet formation models: Dynamical models can explain the broad characteristics of different classes of extra-solar planetary systems. These models rely on two key processes: orbital migration and dynamical instabilities. Migration and instabilities are each important in different regimes: among Earth-sized or larger planets as well as for gas giants systems.

The Solar System's origins: Three current models can match the large-scale properties of the inner Solar System (Fig. 1): the "Grand Tack" [1], "Low-mass asteroid belt" [2,3], and "Early Instability" [4] models. Each model proposes a mechanism to explain specific characteristics of the inner Solar System such as the large Earth/Mars mass ratio and the asteroid belt's orbital and compositional structure. Migration and instability remain central elements of each model. We discuss the strengths and weaknesses of each formation model and their possible Achilles heels.

Implications: We paint a picture of the key steps in planet formation, focusing on the formation times and water contents of potentially habitable rocky planets.

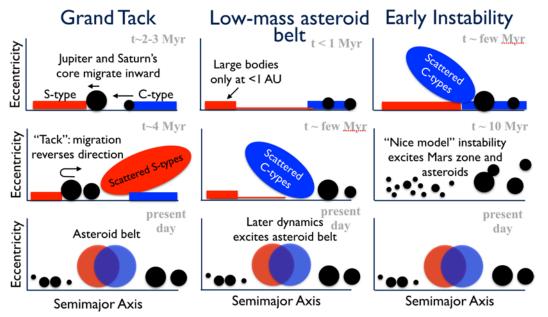


Figure 1. Three competing models for the early evolution of the inner Solar System. Each can match the present-day inner terrestrial planets and asteroid belt. Inward scattering of C-type material is a simple byproduct of giant planet formation and happens in all models [5].

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FORMATION OF TERRESTRIAL PLANETS: CONSTRAINTS FROM ISOTOPIC COMPOSITIONS OF PLANETARY MATERIALS

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Planetary formation appears to be a common process within our galaxy. NASA's Kepler mission has identified more than 2,000 exoplanets, some of which are Earth-size and orbit in the habitable zone around Sun-like stars within our galaxy (e.g., [1]). In 2017, the first interstellar asteroid 11/2017 U1 (aka 'Oumuamua) was detected, but appears unlike any asteroids seen in our Solar System in shape and composition [2]. These results raise ever more questions about planetary formation; the first one to answer is how planetary formation occurred in our own Solar System to make the Earth, a habitable planet harbouring life for at least four billion years.

Observations, numerical simulations and sample analyses can be associated to address the timescales of planetary formation and the source reservoirs of the building blocks of the terrestrial planets and the Moon. From multi-isotopic mass-independent studies of O, and refractory elements such as Cr, Ti, Ca, Sr and Nd, it appears that planetary reservoirs were formed early and separated into two distinct reservoirs (carbonaceous and non-carbonaceous), both showing mixing trends [3-7]. It has been recently suggested that these two reservoirs may have been isolated by the formation of Jupiter within 2 My after CAIs [8]. We still have not identified a unique meteorite group or mixture of meteorite components in our collections matching the bulk Earth's elemental and isotopic compositions [6, 9]. This suggests that Earth may have been made from a mixture of objects that may have formed in different regions of the disc, and some of them may not just be sampled. For many elements (except for Si), however, Earth's isotopic composition is closest to enstatite chondrites, and especially the EL3 sub-group, compared to other meteorite groups, and this for the main and late accretion periods [9-12]. The Earth and the Moon also share strong isotopic similarities [9]. The origin of nucleosynthetic anomalies in siderophile elements such as Mo and Ru (siderophile elements) has provided constraints on the source of the late veneer, and by extension of planetary volatiles, which are critical players for the origin of the atmosphere and life. The ¹⁰⁰Ru anomalies argue against a carbonaceous chondrite origin for the late veneer, while H, C, and N studies indicate the opposite [13]. Volatiles, if from a carbonaceous chondrite source, would thus have to be accreted before the late veneer occurred. Cometary objects cannot be excluded for the origin of noble gases, but they do present a problem for water because of their distinct D/H when compared to Earth [14, 15]. It appears that many differentiated planetesimals, including iron meteorites, have formed before the chondrite parent bodies [16] and could represent other contributors. While iron meteorites have lost their silicate mantles, IAB irons uniquely share their Mo and Ru isotopic compositions with Earth [17-19]. We need to elucidate if they are materials enriched in s-process nucleosynthetic components within the inner Solar System, such as for Venus and Mercury, if the Earth and the Moon progenitor Theia may have grown from similar building blocks or were fully homogeneized, and what the timing and origin of volatile accretion were on Earth and other planets.

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ISOTOPIC CONSTRAINTS ON THE ORIGIN AND EVOLUTION OF PLANETARY ATMOSPHERES G. Avice¹, ¹California Institute of Technology, GPS division, 1200 E. California Blvd, Pasadena, CA 91125, USA, <u>gavice@caltech.edu</u>

Introduction: The presence of water on Earth is a key element of Earth's habitability. However, the Earth probably accreted inside the snow line implying that its forming material was probably relatively volatile-poor. Volatile elements at the Earth's surface were thus probably delivered by late accreting volatile-rich material such as carbonaceous chondrites or comets. In this context, noble gases are excellent physical tracers [1,2] and can answer fundamental questions: i) What was the delivery mix (Solar/Chondritic/Cometary) to planetary atmospheres?; ii) To what extent are silicate portions of terrestrial planets degassed or preserved?; iii) How much of the atmosphere was lost by atmospheric escape and what is the timing of this escape? A long-standing issue in noble gas geochemistry is the so-called "xenon paradox". On Earth and Mars, xenon, the heaviest noble gas seems to present a depletion relative to the Chondritic elemental pattern and a strong enrichment of heavy isotopes relative to light isotopes by 30-40 ‰ per atomic mass unit.

Outline of the talk: I will present how recent results obtained by space missions and measurements of terrestrial samples help to put constraints on the origin and early evolution of volatile elements on terrestrial planets. The first part of the talk will be dedicated to a presentation of noble gas evidence regarding the origin of planetary volatiles and planetary atmospheres. Recent results [3,4] from the ESA Rosetta mission around comet 67P/C-G will be reviewed in the context of the possible delivery of volatile elements to planetary atmospheres by water-rich bodies. The second part of the talk will present the state of knowledge on the evolution of the isotopic composition of atmospheric Xe on Earth [5,6,7]. Results show that this composition evolved from the primordial component U-Xe to the modern composition during billions of years. The evolution stopped around 2 Ga ago. These observations suggest a selective escape of Xe accompanied by isotopic fractionation. Xe escape could be linked to prolonged escape of hydrogen to space. The isotopic composition of atmospheric xenon could be an indicator of the progressive oxidation of the Earth's surface environment [8]. However, a similar depletion pattern and isotopic fractionation of Xe in the Mars atmosphere raises questions given the very different physical parameters for the two planets. In this context, measuring the elemental and isotopic composition of noble gases in the Venus atmosphere is of high priority to further extend comparative planetology in noble gas geochemistry and to understand why Venus evolved differently leading to very different environmental conditions.

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ONSET OF LATE ACCRETION TO THE INNER SOLAR SYSTEM – CONSEQUENCES FOR THE FIRST HABITATS

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The timescale for late accretion to the terrestrial planets is poorly known. Nectarian, Tolstojan and Noachian (pre-3900 Ma) terranes are the oldest and most heavily cratered on the Moon, Mercury and Mars. The latter two have crater densities vs. time comparable to the ancient highlands of the Moon as established from direct sampling in the Apollo and Luna missions. The earliest thermal events recorded in asteroidal meteorites show evidence for crust formation and subsequent continuous resetting by impacts of high closure-temperature radiogenic systems such as U-Pb and Pb-Pb up to about 4.43 Gyr. This cooling age profile for asteroids pre-date absolute ages for the last time the crusts of Earth (ca. 4.40 Gyr), Moon (ca. 4.42 Gyr) and Mars (ca. 4.43 Gyr), as established by U-Pb zircon geochronology, could have experienced wholesale melting by bombardment. Younger ages defined by the relatively low closure-temperature ⁴⁰⁻³⁹Ar geochronological system likewise display a continuum of ages, but these only pick up at ca. 4.48 Gyr and then extend to later times up to as young as 0.25 Gyr ago. Here, we couple dynamical models of late accretion, with ages compiled from radiogenic systems with variable sensitivity to age-resetting by thermal metamorphism, to show that subsequent to Moon formation the flux of comets to the inner solar system reset ages of planetary crusts to ca. 4.45 Ga. Concurrent bombardment by leftover planetesimals continued to impact the inner solar system following a smooth (monotonic) decline in flux afterwards. We describe the dynamical basis of this phenomenon in the context of giant planet migration and assess the likelihood that a biosphere could have been established – and continue to survive – beginning about 150 Myr after solar system formation.



CRITICAL BIOGENICITY TESTS FOR ANCIENT MICROFOSSILS

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Reconstructing the nature and habitat of early life is a difficult task that strongly depends on the study of rare microfossils in ancient rocks. As we trace this record of life back in deep time, however, three obstacles are encountered; 1) microorganisms lack sufficient morphologic complexity to be distinguished from each other and from certain abiologic microstructures, 2) early habitats of life were dominated by hydrothermal processes that can generate abiologic organic microstructures, and 3) the ancient rock record has been metamorphosed causing variable degradation of microbial cells and introducing further abiologic artifacts. Overall, we are thus left with an incomplete record of life that becomes increasingly controversial as we study progressively older rocks.

Here an overview is given of the transformations that occur in microbial cells during silica entombment and prograde metamorphism. Recent results of experimental silicification of microbial cells are presented, showing that specific cell components are better preserved than others, leading to bias in the microfossil record.

Furthermore, a critical assessment is made of abiologic carbonate-silica biomorphs. These crystalline aggregates with life-like morphologies can self-assemble in alkaline silica-saturated fluids that are generated during low-temperature hydrothermal serpentinization of ultramafic crust. Hydrocarbons, formed from e.g. hydrothermal Fischer-Tropsch type synthesis, could adsorb onto these biomorphs, leading to structures that resemble microfossils. Although this process has been extensively cited in literature, so far only one specific filamentous biomorph has been discussed for the interpretation of Archean microfossils. We present the results of witherite biomorph synthesis experiments in silica saturated solution, for an array of pH values and barium concentrations. A wide range of life-like structures is produced, from fractal dendrites to complex shapes with continuous curvature. Biomorph morphology appears to be strongly dependent on the pH of the system, potentially limiting the diversity of early Earth environments in which specific morphologies can be encountered. Other important pseudofossils in rocks are interstitial micro-spaces, that are morphologically complex and that can be filled with hydrocarbons. As with biomorphs, a variety of shapes can be present, showing that the study of individual morphologies is a poor criterion for biogenicity.

Based on these problems, we propose a new general approach for fossil recognition: the morphometric description of entire populations of microstructures (spatial distribution, size distribution, and morphologic descriptor parameters). A critical comparison is made between populations of modern microorganisms, silica-witherite biomorphs and interstitial space fillings. It is shown that statistical morphometry of populations successfully distinguishes fossils from pseudofossils, indicating a strong potential for tracing ancient life on Earth, and possibly the search for traces of life on Mars.



EARLY DIAGENETIC CHERT AS A WINDOW INTO MICROBIAL LIFE AND ENVIRONMENTS

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Early diagenetic chert has long held promise as a critical window into early life on Earth. Increasingly, analytical advances have been aimed at determining (1) the extent to which preserved organic matter is indigenous to our most ancient samples, (2) the origin of preserved organic matter, and (3) the potential for associated chemistry to serve as biochemical indicators of habitability.

Here we explore the potential for early diagenetic chert from younger Proterozoic successions where the biogenicity of preserved organic material is not in question—to further inform our understanding of early diagenetic chert as a target for astrobiological studies. As an example, we will use early diagenetic chert from the 1.1 Ga Angmaat Formation, northern Baffin Island, Canada. Angmaat Formation chert exquisitely preserves a peritidal microbial ecosystem that includes distinct filamentous and coccoidal microbial assemblages, that are arranged across discrete environments (e.g., Knoll et al., 2013), and which are preserved over a broad range of taphonomic states.

Such exquisite preservation of microbial substrates, however, allows us to be to address questions beyond that which involve the preservation of discrete microfossils. We will show the relationship between depositional fabrics preserved within early diagenetic chert and how these fabrics can better inform our understanding of fabric generation within non-silicified phases. We will then explore the range of preserved mat fabrics and associated silicic and non-silicic phases to help constrain the environments of microbial growth and preservation, and see whether these environments are reflected in the composition of extracted organic matter. Finally, petrographic analysis of the chert itself will be used to explore the mechanisms of early diagenetic silicification and the implications for organic matter preservation.

We hope, over the next few years, to build collaborations to further the analysis of these spectacular chert samples. Specifically, we believe that the exquisite preservation of microbial communities within Angmaat Formation chert provides a critical end-member in our understanding of how microanalytical techniques can further our understanding of chert as an astrobiological target.



"TRUE" AND "FALSE" MICROBIAL BIOSIGNATURES IN ASTROBIOLOGY: LESSONS FROM ORGANOMINERALIZATION AND BIOMINERALIZATION EXPERIMENTS

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For more than three quarters of its history, life on Earth was exclusively microbial, and it is thought that if life should exist or have existed elsewhere in our solar system, it would share characteristics with a microbial form. The identification of microbial biosignatures in rocks and ices is thus crucial for our understanding of the origin and early history of life on our planet, as well as the discovery of life elsewhere in the solar system. This task is complicated by the fact that non-biological processes can produce microscopic objects, called biomorphs, that closely resemble microorganisms.

Here we will present a new class of biomorphs formed through the reaction of hydrogen sulfide with dissolved organic molecules, *i.e.* through an organomineralization process. These biomorphs have spherical and filamentous shapes (Figure 1), and are composed of elemental sulfur encapsulated within an organic envelope [1]. We will show that they can form in the presence of simple, prebiotic types of organics, under geochemical conditions that can be found in a wide range of modern and ancient environments. This organomineralization process might be at the origin of elemental sulfur particles found in a sulfide-rich subsurface environment (Frassassi caves, Italy). These new results emphasize the likelihood that organic-sulfur biomorphs might form or have formed in different environments that are relevant to astrobiology. We present data from silicification experiments of these biomorphs, compared with actual sulfur bacteria, showing that If preserved in the rock record (*e.g.* in cherts), these "false biosignatures" would most certainly be interpreted as microbial fossils.

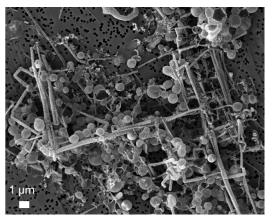


Figure 1: filamentous organic-sulfur biomorphs formed through chemical organic self assembly in the presence of sulfide.

The question is then: can we find examples of "robust" microbial biosignatures? I will use the example of calcium-phosphate forming bacteria to show that microbial biomineralization can sometimes produce very specific features that can be preserved in ancient rocks. These signatures can be revealed by an approach combining the use of model bacterial systems in the laboratory [2] and the nano-scale investigation of fossil bacteria in the rock record [3].

References:

[1] Cosmidis J. & Templeton A. (2016) *Nature Communications*, 7, 12812. [2] Cosmidis J. et al. (2015), *Frontiers in Earth Science*, 3, 84. [3] Cosmidis et al. (2013), *Geobiology*, 11, 139–153.



ISOTOPIC SIGNATURES OF GLOBAL-SCALE BIOLOGICAL ACTIVITY

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The fingerprints of biological activity on Earth are preserved in the rock record. Some morphological, chemical and isotopic "fossils" could be a direct evidence for the existence of life. On the other hand, global-scale biological activity is critical to shape material cycling on the surface of planet Earth, which can thus be traced through a geochemical study. An example is carbonate carbon isotopes which have been fractionated compared to mantle carbon at least since 3.8 Ga. This fractionation shows that the carbon entering into the atmosphere-ocean system was partially transferred into ¹³C-depleted organic carbon. Thus, the observed ¹³C-enrichment in the carbonate rocks possibly suggest that biological carbon fixation has been operated and influenced carbon cycling in a global-scale since 3.8 Ga.

To extend this view, we have studied sulfur isotopes of Archean granitoids, which may provide an alternative view of global-scale microbial sulfate reduction. Previous studies on Phanerozoic granitoids suggested that seawater sulfate is transferred into granitoids via interaction between seawater and oceanic crust and subsequent subduction at the convergent plate boundary, in which dehydrated S-bearing fluid from the oceanic plate was responsible for the magmatism forming granitoids. Our high precision quadruple sulfur isotope analyses $({}^{32}S/{}^{34}S/{}^{36}S)$ of Phanerozoic granitoids confirmed the preservation of seawater-derived signals in granitoids. Furthermore, the same analysis of Archean granitoids including the oldest one from the 4.0 Ga Acasta Gneiss Complex extended this view and for the first time showed that some Archean granitoids possess sulfur with a negative $\Delta^{33}S$ value, which probably originated from seawter sulfate at that time. The observed fractionation of these granitoids suggests that the Archean seawater sulfate would have been consumed by sulfate reducers. These new data provide the oldest evidence indicating that microbial activity would have been active and influence the Earth's global S cycling probably since 4.0 billion years ago.