Universal biosignatures for life detection

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Finding a form of life that is not of terrestrial origin is one of the great frontiers of human endeavor because it would tell us as much about other forms of life as it would tell us about ourselves. But how would we recognize alien biochemistries? Do we understand enough about what constrains a self-sustaining chemical system that undergoes Darwinian evolution to be able to distinguish biotic from abiotic chemistries? I argue that the requirement of information storage and processing in systems of replicating molecules leaves an unambiguous biosignature, revealed by unexpected relative abundances of the "alphabet molecules". I show that this biosignature cannot be missed when using amino acids or carboxylic acids as the alphabet molecules to detect terran life, and that such a biosignature can also easily and robustly detect an artificial life form that lives within computers and has been used extensively for evolutionary research. This work suggests that planetary missions searching for life should focus on measuring relative abundances of classes of molecules that could conceivably be used as an alphabet, given the local chemistry.

Is it Possible to Build a Scientific Theory of the Origin of Life?

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After sixty years of experimental work on the origin of life, there is still no agreement on a conceptual framework describing the process. The importance of contingency is favored by part of the community whereas others support a strong influence of determinism. In addition, a whole spectrum of combinations of the two factors has been proposed. A new approach is put forward. It starts from the prerequisite that any *scientific* description of the process must avoid the occurrence of highly improbable events and leads to define constraints on the process that can be used to build a self-consistent scenario involving stages of increasing levels of organization. This view requires that the intermediate stages take advantage of a kind of stability that is different from thermodynamic stability and that is identified as Dynamic Kinetic Stability (DKS) – the stability form introduced by Addy Pross that is specific of entities that can multiply themselves. Combining this kinetic approach with the necessity of far-from-equilibrium conditions leads to define semi-quantitative constraints on origin of life scenarios. One of these constraints is the need for the evolving system to continuously expend a cost of irreversibility that cannot be converted into chemical work, which has to be taken into account in future investigations in the field.

Compositional lipid assemblies: non-RNA scenario for life's early evolution

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Life's origin is about how sufficient chemical complexity emerged on early earth to afford replication. The graded autocatalysis replication domain (GARD) model (1), in the realm of the lipid world scenario (2), offers a novel route for these events, presumed to have taken place much before the advent of complex biopolymers, such as RNA. In this framework, non-covalent assemblies of diverse amphiphiles, e.g. multi-component lipid micelles or vesicles, can acquire adequate endogenous complexity and harbor considerable inter-assembly variation. Our computer simulations show that GARD assemblies carry and transmit compositional information through homeostatic growth, mediated by a set of catalyzed chemical reactions akin to metabolism followed by random fission. Key in GARD dynamics are *composomes*, spontaneously-forming replication-prone states of compositional dynamics. We have recently demonstrated that composome populations resemble the much-studied RNA quasispecies. We further showed that such GARD species display a significant measure of Darwinian selection and evolution, particularly when their catalytic networks are enriched in mutual-catalysis as opposed to self-catalysis (3). Finally, we found that composome populations portray ecological dynamics that fit the logistic equation, often used to analyze species transitions. Thus, the GARD formalism allows one to outline a well-defined chemically-rigorous path from random chemical environments ("primordial soup") to replicating and evolving protocellular structures, without a prerequisite appearance of RNA-like catalytic replicators. Current GARD studies seek a quantitative delineation of the transition from compositional information to polymer-based sequence-based information, thus supporting the concept of metabolism as a precursor for RNA world.

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Let us go to the basics

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Abstract:
There are several basic questions about the Origin of Life, e.g., whether the first organisms were autotrophic or heterotrophic, whether metabolism was earlier or replication was. Is there any rational point of view to answer (or to avoid) at least partially such questions? Starting with how complex systems must be understood, I wish to discuss a consistent picture of the Origin, which might question some common-sense ideas.

Creation of possible living organisms to study an early life

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It has been widely believed that every modern cell on the earth have been evolved from hypothetical common ancient cells, called as Commonotes (Yamagishi et al. 1997) or LUCAs (Koonin 2003). The Commonotes provided a start point for the biological evolution of modern cells 3.5 to 3.8 billion years ago (Fig. 1). Differ from protocells (Szostak et al. 2008), it is thought that the Commonotes had already possessed some kinds of basic cellular functions that we can now find in modern cells, e.g. protein synthesis using genetic information, cell membrane, energy acquisition, etc. An attempt to resurrect the Commonotes in laboratory has been implemented within the framework of Minimal Cell (Luisi et al. 2006) research. On this research line, we have specially focused on the properties of cell membrane.

In this symposium, I will show a constructive model of the minimal cell that can produce phospholipid within the vesicle compartment. Because the produced phospholipid is the precursor of the vesicle-forming lipid, this would be a plausible model of the self-reproducible minimal cell (Kuruma et al.). Additionally, We have also constructed an artificial cell organelle that can produce ATP by light irradiation. This is composed of a light-induced H^+-pump and ΔpH-driven ATP synthase. Energy acquiring is important property of autonomous cell. We think this will be an interesting cell component not only for the commonotes but also for construction of artificial cell. We would like to discuss how such synthetic approach can contribute to the study of origin of life.

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The Grand Tack scenario for the formation of terrestrial planets. Implications on water delivery to the Earth and on the age of the Moon.

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I will review the motivation and the basic aspects of the Grand Tack scenario for the formation of terrestrial planets. The Grand Tack scenario is the first model that couples giant planet migration during the gas-disk phase to the terrestrial planet accretion process. By assuming a reversal in Jupiter's migration (or tack) at 1.5 AU, the Grand Tack scenario explains in a natural way why there is no giant planet in the inner Solar System, the high mass ratio between the Earth and Mars and the structure of the asteroid belt. By tracking the particles that are initially located in between or beyond the giant planets orbits and assuming that they represent planetesimals of composition similar to carbonaceous chondrites, we compute that the Earth would have accreted from them about 2% of its mass, enough to explain the terrestrial water and noble gases budget. We also studied in details the dependence of the terrestrial planet accretion process on two parameters: the ratio between the total masses in planetary embryos and in planetesimals and the individual mass of the embryos. We found that the former governs the timescale of accretion of the Earth, i.e. the statistical timing of the last giant impact. Instead, the second parameter governs the accretion timescale for Mars. We also found a correlation between the time of the last giant impact and the mass of the Late Veneer accreted by the Earth. The latter is constrained to be 0.5-1% of an Earth mass, from the abundance of Highly Siderophile Elements in the terrestrial mantle. Using this constraint we deduced that the last giant impact on Earth (the Moon forming event) occurred between 60 and 120 My after "time 0" (the formation time of the first solar system solids).

Early thermal events of the inner solar system from zircon geochronology, geochemistry, and thermometry of asteroidal meteorites and lunar rocks

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Understanding the origin and evolution of the planets requires better constraints on the timing and intensity of early thermal events in the asteroid belt and Moon, including the proposed "Late Heavy Bombardment" (LHB) at ca. 3.9 Ga [1]. Both the eucrites (from asteroid 4 Vesta) and lunar impact breccias contain accessory minerals (e.g. zircon, apatite, baddeleyite, zirconolite) with U-Pb ages that may not have been wholly re-set by thermal events subsequent to their original formation; many of these pre-date the LHB epoch and yield complex histories perhaps associated with multiple shock events [2-4] of uncertain affinity. Therefore further detailed geochronological analyses are warranted to uncover a cryptic record of "pre-LHB" bombardments. Zircons are useful in this regard because they are oft-quoted as the most reliable chronometers despite (sometimes significant) thermal metamorphism. A suite of criteria used to elucidate the petrogenetic history of a zircon include: determination whether they are the products of a purely crustal igneous process; crystallized from impact melts; or experienced diffusion-controlled age resetting from impact shock heating resulting in the partial re-setting of pre-existing igneous zircon. Geochemical tools to distinguish between these different scenarios include U-Pb geochronology, trace element geochemistry, Ti-in-zircon thermometry [5] and zircon-melt partition modeling [6]. Ultra-high resolution (sub-μm) U-Th-Pb depth profiles in eucritic zircons reveal different age domains correlative to mineral chemistry in cores and mantles within individual zircons. Results from eucrite zircons confirm previous ages determined for the solidification 4 Vesta's crust within a few million years after the formation of CAIs (4561±13 Ma), while younger ages may be the result of either shock metamorphism via impact heating or are associated with protracted basaltic magmatism. Furthermore, U-Th-Pb-Ti abundances for 106 lunar zircons from lunar impact breccia 14311 show three distinct age populations of 4314 ± 11 Ma, 4214 ± 10 Ma, and 4007 ± 16 Ma. Thermometry results reveal temperatures that range from 700-1200 ^{o}C. A larger majority of zircons from the youngest population yield slightly higher temperatures compared to the older groups and are within the range of modeled impact melt values for the Moon [6]. Taken together, U-Pb ages, geochemistry and partition modeling suggest oldest zircon population represents primary igneous crustal formation at ca. 4.3 Ga, while the 4.2 Ga zircons may be a mixture of igneous and impact-produced zircons. Impact-generated or altered lunar zircons at about 4.0 and 4.2 Ga coincide with "LHB" and "pre-LHB" events reported in other radiogenic systems [7], other zircon ages from lunar impact breccias [2-4], as well as the oldest terrestrial zircons [8]. These results support a longer period of bombardment akin to the proposed "Sawtooth" model [9].

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The origin of solar system water as recorded by its D/H ratio.

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The isotopic composition of hydrogen (expressed as the D/ H ratio) is a geochemical tracer of the origin of water in the solar system (Robert 2006). Primitive carbonaceous chondrites (CCs), presumably the carriers of most volatile elements in terrestrial planets, have presumably recorded the D/H ratio of water in the protosolar nebula (PSN). Because of the slowness of silicate alteration by water vapor in the PSN, the formation of the clays that are found in most CCs, is attributed to reactions with liquid water circulating in parent bodies CCs. This water was presumably incorporated as ice along with rock during accretion. Therefore, the measured distribution of the D/H ratios in bulk CCs is generally thought to reflect that of accreted water ice. This distribution is reported in the Figure 1 along with the distribution in Interplanetary Dust Particles (IDPs); the domain defined by the comets is also shown for comparison.

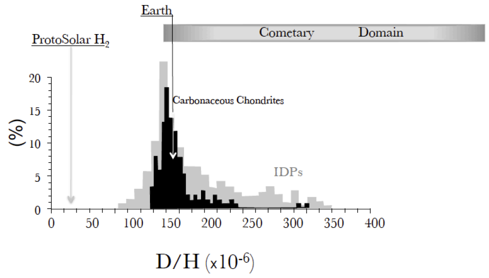

Figure 1 : D/H enrichment histogram showing the enhancement over the protosolar value of the D/H ratio on Earth (see text), in CCs (Carbonaceous Chondrites), in IDPs (Interplanetary Dust Particles).

The distribution which is skewed to heavy isotopic compositions, has a mean value almost indistinguishable from the bulk Earth D/H ratio (149±3 x10^{-6}). Therefore this distribution points towards a chondritic source for terrestrial water rather than a cometary or solar source (Bockellée-Morvan *et al.*, 1998, 2012). This interpretation is also accounted by collisional models where terrestrial planets accreted from embryos (Morbidelli *et al.*, 2000).

Several issues remains nevertheless open, namely: (i) why the chondritic D/H ratio distribution is different from that of comets ? (ii) why the D/H ratio of water is different from that of the PSN molecular H_2 ? (iii) Why the PSN water D/H ratio is not homogeneous in the solar system? Recently several solutions to these issues have been proposed in the literature (Ceccarelli C. and Dominik C., 2005; Remusat *et al.*, 2006; Jacquet et Robert, 2013). They will be presented in this talk along with their caveats.

Recent analytical evidences show that the pristine water embedded in meteorite parent bodies have exhibited much larger variations than actually measured in CCs or in comets (Alexander *et al.*, 2012; Piani *et al* 2012). The interpretation of such an isotopic heterogeneity is qualitatively accounted for by PSN models where water vapor re-equilibrates isotopically with the protosolar molecular H_2 (Drouart *et al.*, 1999; Mousis *et al.*, 2000; Yang *et al.*, 2013). We will show that the presently available theoretical models describing this isotope exchange in time and space, are still incomplete.

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The rates of icy grains filtered by planetesimals and accreted by planets - A possible mechanism to control water fraction of the Earth

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Detailed radiative transfer calculations of thermal state of protoplanetary gas disks, from which planetary systems are formed, show that the snow line inevitably goes inside of the Earth's orbit (1AU) during its evolution.

Then, it is expected that huge amount of icy grains condense around 1AU and consequently, the Earth should become totally wet. How to realize actual "dry" Earth is a serious problem.

We point out that icy grains first condense in outer regions
of the disks. We have calculated the rate of the icy grains filtered out by lanetesimals until they arrive at 1AU to evaluate how much icy grains are accreted onto the protoplanets around 1AU.

Through these calculations, we discuss how the amount of water in the Earth delivered by icy grains is controlled, based on planet formation theory.

On the radius of habitable planets

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The conditions that a planet must fulfill in order to be habitable are not precisely known. However, it is comparatively easier to define conditions under which a planet is very likely not habitable. Finding such conditions is moreover important as it can help to select, in an ensemble of potentially observable planets, which ones should be observed in more details for characterization studies.

Assuming, as in the case of the Earth, that the presence of a C-cycle is a necessary condition for long-term habitability, we derive, as a function of the planetary mass, a radius above which a planet is likely not habitable. For this, we compute the maximum radius a planet can have in order to fulfill two constraints: surface conditions compatible with the existence of liquid water, and no ice layer at the bottom of a putative global ocean. We demonstrate that, above a given radius, these two constraints cannot be met.

For this, we compute internal structure models of planets, using a 5-layer model (core, inner mantle, outer mantle, ocean and atmosphere), for different masses and composition of the planets (in particular Fe/Si ratio of the planet). Our results show that for planets in the Super-Earth mass range (1-12 Mearth), the overall maximum that a planet can have varies between 1.8 and 2.3 Rearth. This radius is reduced when considering planets with higher Fe/Si ratios, and taking into account irradiation when computing the gas envelope structure.

Tar, Water, and Entropy.
Three Paradoxes Obstructing Emergence of an RNA World

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While contemporary molecular biology supports an episode of life on Earth where RNA was the only encoded component of biological catalysis, five paradoxes prevent our concluding that the RNA world started terran life.
(a) The Tar Paradox. Organic molecules, absent biology, inherently devolve into "asphalts", not building blocks for RNA.
(b) The Water Paradox: Even if devolution is avoided, building block assembly is "uphill" in water, and any RNA assembled is corroded by water.
(c) The Entropy Paradox. Without building blocks in implausibly high concentrations, the length of RNA plausibly assemblable appears too short to support Darwinian evolution.
(d) The Single Biopolymer Paradox. Genetics places different demands on biopolymers than catalysis, making it hard for one biopolymer to do both effectively.
(e) The Probability Paradox. Ribozymes degrading RNA arise much more frequently than ribozymes making RNA.
Recently, minerals, exotic solvents, distant locales, and supercritical solvents have been hypothesized to resolve the first three of these. This talk will outline experimental work that examines critically these hypotheses.

Was the Requiem for Life on Mars Premature?

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Nearly 18 years ago, David McKay and coworkers[1] argued that Martian meteorite ALH 84001 contained traces of an ancient biosphere on Mars. The excitement from that announcement led to the creation of the National Astrobiology Institute (NAI), and spurred a host of analyses aimed at testing the question about whether life could have existed elsewhere in the universe. In this talk, I will summarize new information gleaned from numerous Martian satellite and rover missions that place interesting constraints on the early environment of Mars, and show that it would have been at least as good a place for the origin of life as was early Earth, if not better. In fact, every scenario proposed for the origin of life on Earth applies equally well to Mars, and the demonstration that meteorites have traveled on low-temperature, low-shock trajectories from Mars to Earth[2] makes interplanetary panspermia plausible[3].

Although some of the evidence presented by McKay et al. now has plausible inorganic interpretations, the debate continues concerning the possible presence of bacterial magnetofossils in the ALH84001 carbonates[4]. The proposed non-biological interpretation[5] centers on the possible *in-situ* decomposition of iron-bearing carbonate to form the magnetite crystals. In terms of the rock magnetic properties, this mechanism leads to a dramatically different remanent magnetization levels that can now be tested using high-resolution scanning magnetic microscopy. The debate about the possibility of ancient life on Mars is certainly not over!

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Deep-sea hydrothermal vent as bottleneck of Hadean Monsters

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Personally saying, I do not very much care about wherever lives, exactly heterogeneous lives unrelated with our ancestors, were born. It is a matter of ‘Origins of Lives’. Possible places and scenarios are possible and we cannot find the absolute truth. In other words, we can make different kinds of origins of lives in the Earth (exactly saying, in laboratories in the Earth) by synthetic technology in the future, which will be not directly relevant with understanding the true origin of life in this planet but will substantiate deep understanding what is life in the Universe. Anyhow, what we can do is to estimate and justify likelihoods of possible scenarios for origins of lives in the Earth, and to prioritize them. For me, however, it is much more fascinating to imagine how such a diversity of possible early lives have connected with our ancestral lives and finally with us, the modern diverse lives. What I am intuitively convinced of is that deep-sea hydrothermal vent was a connecting place for kinds of possible early lives (Hadean Monsters) and our ancestors as bottleneck of the very early evolution. Of course, I also believe that deep-sea hydrothermal vent is the most likely hatchery place for the first lives and the early evolution of our ancestral lives. Hot springs? Mars? They are lots of fun to talk with……

Chemical Disequilibrium, Hydrothermal Vents, and the Origin of Metabolism

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One of the ubiquitous properties of life on Earth, and perhaps of any life elsewhere, is that it utilizes geochemical and electrochemical disequilibria and converts free energy. Planets with a water-rock interface generate disequilibria through water-rock reactions and hydrothermal vent activity in the form of redox, pH, and thermal gradients. The interface between contrasting ocean and hydrothermal fluids also can lead to the formation of self-assembling, inorganic precipitation chimneys (“inorganic membranes”) that may extend the lifetime of active redox potentials and may also concentrate biologically significant reactants as part of the precipitate, possibly allowing for chemical energy sources to be present over long enough timescales to support an emerging biosphere. Some key questions for astrobiology then center on: investigating the geochemical energy gradients produced on wet rocky planets; learning how these abiotic redox and pH gradients may have participated in prebiotic chemistry and the emergence of bioenergetics; and how the conversion of free energy to drive “uphill” reactions at the origin of life could have proceeded using only geochemically available inorganic components. I will discuss our progress on simulating hydrothermal systems on the early Earth and other wet rocky worlds, focusing on the ability of self-assembling inorganic membranes to mediate geochemical / electrochemical energy and facilitate prebiotic chemistry.

Early life on the anoxic geothermal fields of the primeval Earth

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We have reconstructed the 'hatcheries' of the first cells by combining geochemical analysis with phylogenomic scrutiny of the inorganic ion requirements of universal components of modern cells [1,2]. These ubiquitous, and by inference primordial, proteins and functional systems show affinity to and functional requirement for K^+, Zn^{2+}, Mn^{2+}, and phosphate. Thus, protocells must have evolved in habitats with a high K^+/Na^+ ratio and relatively high concentrations of Zn, Mn and phosphorous compounds. Geochemical reconstruction shows that the ionic composition conducive to the origin of cells could not have existed in marine settings but is compatible with emissions of vapor-dominated zones of inland geothermal systems. Under anoxic, CO_2-dominated atmosphere, the elementary composition of pools of condensed vapor at anoxic geothermal fields would resemble the internal milieu of modern cells.

Experimental studies of abiotic syntheses of biomolecules suggest that specific formation of nucleobases, sugars, and, eventually, even activated, cyclic ribonucleotides with a potential for polymerization could take place in formamide-rich solutions, particularly under the action of UV light and in the presence of borate and phosphorous compounds [3,4].

The exhalations of even modern geothermal fields contain high amounts of ammonia, phosphate, borate and hydrocarbons, so that the anoxic geothermal fields should have been conducive for formation of simple amides and nitrogen-containing organic molecules, including activated nucleotides.

Hence, the anoxic geothermal fields, which we identified as tentative cradles of life by using the top-down approach and phylogenomic analysis, could provide geochemical conditions that were suggested as most conducive for the emergence of life by those chemists who pursued the complementary bottom-up strategy.

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Origin of life on the Hadean Continent

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Where on Earth is the birth place of life? This paramount question has been shrouded in mystery.

For the beginning of life, several critical conditions must be met. For example, there must be a sufficient supply of necessary elements to form the body of living organisms such as clean water, nitrogen, hydrogen, and nutrients with constant energy/material circulation. Where did such place locate on the Hadean Earth?

The answer is on the primordial continent. After the giant impact, whole Earth was melted as well as the Moon. As the planet cooled down gradually, heavy metal components sank into the core and the residual components which remained in the mantle floated on the primordial continent.

There are two critical roles of the primordial continent for life; (1) it provided a lacustrine environment and (2) it provided nutrients (Maruyama et al., 2013).

In the Hadean, chemical composition of ocean was significantly different from that of modern Earth, which was too toxic (high salinity, ultra-high acidity, and ultra-enriched in heavy metal) and impossible for life to live. Therefore, to bear life, the appearance of lakes filled with clean water is necessary. At the same time, primordial continent provided nutrients for the birth place in the Hadean. On this point, hydrothermal system at deep sea floor cannot be the birth place of life. Without a sufficient supply of nutrients from a primordial continent, the life body could not be formed, and organic radical reactions such as metabolism could not proceed (Santosh et al., 2014)

There is no direct evidence of primordial continent on modern Earth, however it is inferable from the geologic record of the Moon. KREEP basalt, enriched in both phosphorous and potassium, which is exposed on the Moon surface had appeared on primordial continent on the Earth and must have played the key role in the origin of life (Maruyama et al., 2013).

A lake with clean water formed on the primordial continent was abundant with nutrients, which established Habitable-Trinity conditions (co-existence of the landmass, ocean, and atmosphere) under the Sun provided a suitable place for the beginning of life for the first time on the Earth (Dohm and Maruyama, in press).

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Origin and evolution of volatiles on Earth

Bernard Marty
CRPG-CNRS

The origin of the Earth's atmosphere is a long debated question, that has recently gained insight thanks to (i) space missions aimed at documenting the composition of the Sun and of planets, (ii) the precise analysis of volatile elements (hydrogen, carbon, nitrogen, noble gases) in the present-day terrestrial mantle and atmosphere/hydrosphere, and (iii) the analysis of ancient (> 3 billion-years old) rocks that have trapped remnant of the primitive atmosphere and of environmental conditions long ago. A review of the current state of knowledge in this domain, as well as new results obtained from our laboratory, will be presented.

Making Proto-planets from melting of chondrites at ultra-high pressures

Steeve Gréaux
ELSI/ Ehime University

Chondrites are stony meteorites carrying materials from the early solar system, which accreted to form primitive asteroids. It is proposed that in the history of our solar system, proto-planets may have been formed by the accretion of primitive meteoritic blocks similar to chondritic materials. If we imagine a proto-planet formed from the accretion of a specific chondritic materials, what kind of layered planet (e.g. core, mantle, crust) can be formed ? and how does it compare to the Earth ?
Here we investigated such questions for the Tagish Lake CI2 carbonaceous chondrite (CC) by means of melting experiments at high-pressure in a multi-anvil press apparatus. The composition of CC in terms of non-volatile elements is close to that of the solar abundances. On the other hand, CC are more Fe-enriched than upper mantle peridotites. We experimented P and T up to 50 GPa and 2500 K, which may correspond to the conditions of deep magma oceans of Mars-to-Earth sized bodies. At all pressures, our results indicate the systematic formation of (Fe,Ni)S metal, which coexist with a Si- and C-rich melt and one crystallizing phase. At P lower than 25 GPa, the majoritic garnet is the first liquidus phase while at 50 GPa, Fe-rich Mg-perovskite is the main phase. Our results are discussed relative to the planetary differentiation processes that may have resulted in the formation of the proto-Earth.

Oxidation state in the early Earth: influence on H, C, S, O, N and other volatiles

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NASA-JSC

The last decade has seen general acceptance of the idea that early Earth experienced a magma ocean stage where the magma ocean could have been as deep as 1500 -2000 km. This environment set not only the concentrations of siderophile elements in the mantle (Ni, Co, Mo, W, etc.), but also many additional elements that are of interest to biochemistry such as H, C, S, O and N. One aspect of the magma ocean scenario that is uncertain (and still causing debate) is the exact oxidation state of the mantle during and after accretion and core formation. Considering a broad range of experimental results on high pressure experimental petrology, it will be shown that a low fO_2 environment will lead to a mantle with high S and N, low H and C, whereas a high fO_2 environment will lead to a mantle with low S and N, high H and C. Additional post-core formation influences on the magma ocean oxidation state include indigenous processes such as pressure dependent equilibria involving melt Fe^{3+} and Fe^{2+}, or high pressure mineral equilibria – i.e., garnet or MgSi-perovskite) as well as exogenous processes such as late chondritic additions. Effort will be made to identify aspects of these scenarios with the greatest uncertainty and thus where we need more work.

Hydrogen in the core

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Kei Hirose
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The melting temperature of the Earth's mantle provides key constraints on the thermal structures of both the mantle and the core. Through high pressure experiments and three-dimensional x-ray micro-tomographic imaging, we show that the solidus temperature of a primitive (pyrolitic) mantle is as low as 3570±200 K at pressures expected near the boundary between the mantle and the outer core. Because the lowermost mantle is not globally molten, this provides an upper bound of the temperature at the core-mantle boundary (T_{CMB}). The upper bounds of T_{CMB} found in this study require that the liquidus temperature of outer core alloy is depressed by >600 K at 136 GPa from that of pure Fe. Such a large depression will be impossible without hydrogen in the core. $Fe_{93.4}H_{0.6}Si_{6}$ (in weight ratio) may be compatible with the low T_{CMB} as well as the 10% core density deficit, although more precise estimate requires the knowledge on liquid density and melting behavior in Fe-H-Si system. 0.6wt% hydrogen in the core corresponds to 80 times seawater in terms of H_2O. A large amount of hydrogen in the core may have been incorporated into metals from hydrous magma ocean at the time of core formation.

Early Earth Differentiation and the Creation of a Recognizable World

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Mars, Mercury and the Moon have surfaces dominated by ancient (> 4 Ga) terranes whereas Earth and Venus have predominantly young surfaces, likely for very different reasons. Samples from Mars and the Moon reveal the importance of extreme global differentiation events, likely magma oceans, shortly following their formation. On Earth, the primary signatures of early differentiation are the siderophile element abundance and W isotopic composition of the mantle that reflect core formation, and the difference in Xe isotopic composition between atmospheric and mantle Xe caused by outgassing from the mantle while the short-lived radioactive isotope ^{129}I was still extant. Unlike Mars and the Moon, the evidence for early differentiation of the silicate Earth is subtle and preserved in only a handful of Eoarchean to Hadean crustal fragments on Earth. Why is this signature of terrestrial early differentiation so muted? Did Earth not experience a magma ocean episode during its formation? Did the physical conditions of magma ocean evolution on a planet the size of Earth force equilibrium instead of fractional crystallization of the magma ocean? Surprisingly, the oldest crustal terranes on Earth suggest that the temperature profile of at least the outermost Hadean Earth was not dramatically different from the present world. For example, the Nuvvagittuq supracrustal belt in northern Quebec consists of a sequence of volcanic rocks, some of which were erupted into liquid water (lakes, oceans?), whose compositional stratigraphy is similar to that of modern intra-oceanic volcanic arcs. Whether this means that plate subduction was occurring in the Hadean will remain a topic of debate for some time, but the evidence that Earth's surface at 3.8 Ga or older was cold enough to allow the presence of liquid water, and that the shallow mantle was characterized by a geotherm not dramatically different than the present day is inescapable. The volcanic record from the Hadean through the Archean thus is consistent with the suggestion by Korenaga (2006) that the temperature in the shallow mantle may have peaked at 3 to 3.5 Ga after rising from cooler conditions in the Hadean. Tracking the reduction in variability in ^{142}Nd/^{144}Nd in mantle-derived rocks through the Archean suggests that a significantly heterogeneous mantle left after initial Earth differentiation was being homogenized by mantle convection from 4 to 3 Ga, perhaps reflecting the onset of plate tectonics and crustal recycling in this early era of Earth evolution.

Early Evolution of Rocky Exoplanets in the Habitable Zones of M dwarfs

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The Hadean era is an important phase of the Earth's evolution history because events occurred during this time largely determined the bulk composition of the planet's volatile inventory, setting up the stage for the planet's future evolution. M dwarfs are the most important targets of habitable exoplanet search missions and projects in the coming decade. Our current knowledge of M dwarfs indicates that the early evolution of rocky planets in the liquid water habitable zones (HZ) of these stars should be rather different from that of the Hadean Earth. More specifically, rocky planets in the HZ of M dwarfs experience strong XUV radiation and almost continuous bombardment of stellar wind, which could lead to substantial mass loss from these bodies. In this talk we will discuss the early evolution of rocky planets in the HZ of M dwarfs and compare them with Hadean Earth.

Rocks, water, impacts, life and the Hadean-Eoarchean transition on Earth

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The geochemical and cosmochemical record of our solar system is the baseline for exploring the question: "when could life appear on a world similar to our own?" Data arising from direct analysis of the oldest terrestrial rocks and minerals from the first 700 Myr of Earth history – termed the Hadean Eon – inform us about the timing for the establishment of a silicate+metal world such as Earth that is eminently suitable for life. Liquid water is the key medium for life. The origin of water, and its interaction with the crust as revealed in the geologic record, guides this exploration. From the time of primary planetary accretion to the start of the continuous rock record at the Hadean-Eoarchean transition (ca. 3850 Myr ago), our planet experienced a waning bolide flux that partially or entirely wiped out surface rocks, vaporized oceans, and created transient serpentinizing atmospheres. Arguably, "Early Earths" across the galaxy may start off as ice planets due to feeble insolation from their young stars, occasionally punctuated by steam atmospheres generated by cataclysmic impacts. Alternatively, early global environments conducive to life spanned from a benign surface zone to deep into crustal rocks and sediments; models for early environments are strongly dependent on early intense greenhouse atmospheres. In some scenarios, early biospheres may benefit from exogenous delivery of essential bio-elements via leftovers of accretion, and the subsequent establishment of large long-lived hydrothermal systems from the largest impacts.

I will review what is known about the early availability and long-term stability of liquid water, gross evolution of the basalt-granite dichotomy, and speculate on P-T conditions at or near the surface suitable for sustaining biological activity. I will argue that life could have emerged in or on Earth within ca. 150 Myr after its formation. Our understanding of the thermal histories and chemical transformations of the crusts of early Earth, Moon, Mars and asteroids have accumulated to the point where it is now feasible to deduce the habitable potential of the nascent solar system and to place some upward constraints on the timing of life's appearance.

Evolution of Commonote(s): History revealed by genetic engineering.

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All of the living species on Earth have been evolved from the organism called LUCA (Last Universal Common Ancestor), senancestor or Commonote (Yamagishi et al. 1998). We defined the Commonote as the last and the latest common ancestral species, which shared the gene pool, of all the extent organisms. The Commonote has separated into the two groups: Bacteria and Archaea + Eucarya.

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. 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 (Akanuma et al. 2013).

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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Deep-time, data-driven discovery in mineralogy:
Evidence for the co-evolution of life and minerals

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Discovery in geochemistry relies principally on induction and deduction—approaches to reasoning that focus on observation, modeling, and predictive explanations of known natural patterns and phenomena. However, these powerful methods are inherently inefficient at discovering new complex patterns that require multivariate analysis of large datasets or synthesis of diverse types of data. Recognition of global processes associated with the origins and evolution of life, including oxidation of the oceans and atmosphere, diversification of near-surface mineralogy, and co-evolution of the terrestrial geosphere and biosphere, may require decades of integrated geo- and bioscience data. Accordingly, we are developing a deep-time data infrastructure that links trace element and isotope data for rocks and minerals to paleoenvironment, paleobiology, proteomics, and thermochemical data resources. The potential now exists for an alternative "abductive" approach to investigate Earth's co-evolving geo- and biosphere [1-4].

Earth's near-surface environment has evolved as a consequence of selective physical, chemical, and biological processes—an evolution that is preserved in the mineralogical record. Recent studies of mineral diversification through time reveal correlations with major geochemical, tectonic, and biological events, including large-changes in ocean chemistry, the supercontinent cycle, the increase of atmospheric oxygen, and the rise of the terrestrial biosphere. Data on trace element distributions [5] and species diversification [6-8] reveal significant temporal changes in Earth's near-surface oxidation state. Growing data resources also point to new opportunities for applying multivariate statistical methods and adapting visualization strategies for deep-time data. Ultimately, we envision an integrated deep-time data infrastructure—a new kind of open-access "scientific instrument" that may facilitate transformation of current Earth science paradigms.

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Redox evolution before oxygenic photosynthesis

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Redox evolution of the ocean and atmosphere system is a key to understand early evolution of biosphere. S-MIF has potential to monitor chemistry of the Earth's early atmosphere, though the mechanism of the S-MIF is still poorly understood. Previous laboratory experiments indicate isotopic anomaly can be produced via photolysis of SO_2, depending largely on UV wavelength and partial pressure of SO_2, though none of these experiments have not yet succeeded to fully reproduce the S-MIF recorded in the Archean sedimentary rocks (e.g., Danielache et al., 2008; Masterson et al., 2011; Whitehill & Ono, 2012). We have developed a new photochemical chamber for determining isotopic effect of the SO_2 photolysis under optically thin condition. The results indicate that the basic character of the S-MIF observed in the Archean record can be reproduced when SO_2 column density is reasonably low. Numerical modeling of the atmospheric chemistry suggests that the observed D36S/D33S trends can be useful for monitoring SO_2 partial pressure and amount of reducing gas (H_2, CH_4 and CO) in the atmosphere on average. In light of the new perspective, we have re-evaluated the geological record of the D36S/D33S ratio with additional analyses of Archean sedimentary sulfides. Based on the magnitude of the S-MIF and the D36S/D33S ratio, the Archean period can be subdivided into four stages, probably reflecting both intensity of volcanic SO_2 emission and concentration of reducing gasses under the O_2-free atmosphere. Particularly, the maximum scatter of D33S values observed in the late Archean (2.7-2.5 Ga) requires high volcanic emission as well as very reducing atmospheric condition in the atmosphere at that time. This may suggest increasing activity of photosynthesis rather made the atmosphere more reducing possibly owing to enhanced primary productivity at the late Archean.

The history of the Mn cycle and the evolution of photosynthesis

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The emergence of oxygenic photosynthesis fundamentally transformed our planet; however, the processes that led to the innovation of biological water splitting have remained largely unknown. From an evolutionary perspective, it is notable that modern biological water-splitting in photosynthesis begins with Mn oxidation in the water-oxidizing complex of photosystem II, suggesting several evolutionary scenarios wherein Mn(II) once played a key role as an electron donor for photosynthesis prior to the evolution of oxygenic photosynthesis. To test this hypothesis, we examined the behavior of the ancient Mn cycle using newly obtained scientific drill cores through an early Paleoproterozoic succession of sedimentary rocks (2.415 Ga) preserved in South Africa. These strata contain the oldest substantial Mn enrichments (up to ~17 wt %), well before those associated with the rise of oxygen such as the ~2.2 Ga Kalahari Mn deposit. Using both bulk and microscale X-ray spectroscopic techniques coupled to optical and electron microscopy and stable carbon isotope ratios, we determined that the Mn is hosted exclusively in carbonate mineral phases derived from reduction of Mn oxides during diagenesis of primary sediments. Additional observations of independent proxies for molecular oxygen—multiple S isotopes (measured in bulk by isotope-ratio mass spectrometry and *in situ* by secondary ion mass spectrometry) and redox-sensitive detrital grains—reveal that the original Mn-oxide phases were not produced by reactions with oxygen, which points to a different high-potential oxidant. These results show that the oxidative branch of the Mn cycle predates the rise of oxygen, and supports the hypothesis that the water-oxidizing complex of photosystem II evolved from a former transitional photosystem capable of single-electron oxidation reactions of Mn.

Light to Life

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I suggest that the early evolution of photosynthetic reactions in microbes was made possible by band gaps in transition metal bearing minerals. The most abundant transition metal in the Archean oceans was, by far, iron. DFT calculations with one iron bearing mineral, siderite ($FeCO_3$), indicate an antibonding orbital at 4.8 eV. Experiments reveal that this orbital can be populated under anoxic conditions in aqueous phase to oxidize the iron, yielding H_2 gas. I will present this and other data pointing a way towards understanding how abiotic, photogeochemical reactions became photobiological reactions in the early Archean oceans.

Early Evolution of Photosynthesis and the Transition to an Aerobic World

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Energy conversion of sunlight by photosynthetic organisms has changed Earth and life on it. Photosynthesis arose early in Earth's history, and the earliest forms of photosynthetic life were almost certainly anoxygenic (non-oxygen evolving). The invention of oxygenic photosynthesis and the subsequent rise of atmospheric oxygen approximately 2.4 billion years ago revolutionized the energetic and enzymatic fundamentals of life. The repercussions of this revolution are manifested in novel biosynthetic pathways of photosynthetic cofactors and the modification of electron carriers, pigments, and existing and alternative modes of photosynthetic carbon fixation. The evolutionary history of photosynthetic organisms is further complicated by lateral gene transfer that involved photosynthetic components as well as by endosymbiotic events. An expanding wealth of genetic information, together with biochemical, biophysical, and physiological data, reveals a mosaic of photosynthetic features. In combination, these data provide an increasingly robust framework to formulate and evaluate hypotheses concerning the origin and evolution of photosynthesis.

Current status of laboratory experiments for artificial creation of oxygenic photosynthesis; elucidation of genetic backgrounds necessary for chlorophyll *a* biosynthesis

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Mechanisms of how oxygenic photosynthesis was established from anoxygenic photosynthesis is critically important for elucidating evolution of early earth, although the mechanism is still under investigation. A critical step for establishing oxygenic photosynthesis may be synthesizing chlorophyll *a*, because oxygenic phototrophs, such as cyanobacteria, use chlorophyll *a*, although anoxygenic phototrophs, such as purple bacteria and green sulfur bacteria, use bacteriochlorophyll(s), as main pigments.

To elucidate what components are required for early evolution of photosynthesis, we have tried to mimic evolution of oxygenic phototrophs from anoxygenic photosynthetic bacteria by direct mutagenesis. Recently, we succeeded to isolate the genetically modified purple bacterium that is capable of synthesizing chlorophyll *a*. For chlorophyll *a* synthesis in the bacterium, genes for photosystem I-type reaction center as well as galactolipid synthesis were pre-requested. This result indicated the coupling arrangement of chlorophyll synthesis, reaction centers, and membrane lipids for establishing oxygenic photosynthesis in the course of evolution.

ELSI-Inspired Model for the Formation and Evolution of Earth's Interior

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One of the loftiest goals of geology is to develop the theoretical tools necessary to establish a reasonable initial state of Earth, such as its composition and temperature profile, and then use material properties and coupled models for Earth's processes to predict the evolution through time to the present day. In practice, this evolution is complicated and is still not well-understood, and there are many uncertainties involved in arriving at a fully self-consistent model for Earth's evolution through time. For example, the style of tectonics in the early Earth plays an important role in many processes, but is not so well-understood and is anyways highly debated. However, there are other constraints that are relatively firm and might be leveraged to help distinguish between uncertain scenarios. One important constraint is conservation of energy, a number that must add up in the sum of interactions between Earth's systems. We are also fortunate enough to be provided with a plethora of information regarding Earth's present temperatures, compositions, and geological structure (i.e., the end state). From this perspective, Earth's history looks like an initial value problem in differential equations, grounded in conservation of energy, and with poorly constrained initial conditions. We can, however, use forward models of Earth's evolution, in concert with inverse-time inferences, and bringing together more constraints than have been leveraged in the past, in order to find solutions for the formation and early evolution of Earth that yield appropriate conditions and consistent structures at the present time.