# Day 1, Tuesday, 30.8.2022

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<sup>1</sup>Carnegie Institution for Science

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# Session 1

14:00 - 14:40

63

### **Keynote**

# When, How and in What Were the Most Volatile Elements Delivered to the Earth?

### Alexander C<sup>1</sup>

<sup>1</sup>Carnegie Institution for Science

In the standard model of terrestrial planet formation, first ~ Mars-sized embryos form by oligarchic accretion of planetesimals, and then on longer timescales the final growth phase is dominated by collisions of embryos. Mars had already reached roughly half its current size within ~2 Ma of Solar System formation. If Mars is typical of embryos, their rapid formation implies that they would have largely formed by accretion of earlier formed planetesimals that, as a result of 26Al decay, would have melted and differentiated. Measurements of achondrites indicate that they generally have very low volatile contents. The meteorite record suggests that planetesimal formation in the inner Solar System ended at ~2 Ma, and those planetesimals that did not differentiate were heavily metamorphosed and degassed. However, dynamical models indicate that the giant planets would have scattered planetesimals from the outer to the inner Solar System as they grew and their orbits evolved. If these scattered outer Solar System planetesimals formed after ~3 Ma, they are likely to have been very volatile-rich. This is the case for the CI, CM and CR carbonaceous chondrites as well as comets, and only relatively small amounts of these objects are needed to account for the volatile inventories of the terrestrial planets. Comparisons of the noble gas abundances/isotopes, and H and N isotopes, suggest that most of the Earth's volatiles were accreted in CIand/or CM-like bodies, with relatively small contributions from comets and solar/solar wind material. The small solar contributions suggests that the Earth did not acquire a primary atmosphere from the solar nebula, placing limits on how big its building blocks were when the gas disk dissipated. If a late veneer is the explanation for the HSEs, S, Se and Te in the BSE, then most of the Earth's volatiles were accreted prior to the Moon-forming impact. Most estimates of the BSE's H and C contents, and all estimates of its N content are much lower than would be predicted for CI/CM-like sources based on the noble gases. Impact-driven loss of early atmospheres that degassed from impact-generated magma oceans is one possible explanation low H, C and N abundances, but this may be hard to reconcile with the much higher and relatively unfractionated CI-normalized abundances of Ne and Ar that have similar solubilities in silicate melts to CO2 and N2, respectively. Possible alternative explanations for any H, C, and N depletions, relative to the noble gases, in the BSE are significant partitioning into the core or hidden reservoirs in the deep mantle. Equally puzzling is the Ne isotopic difference between the Earth's atmosphere (70-80% chondritic, 20-30% solar) and primitive mantle (solar-like). Taken at face value, it would seem to imply that the bulk of the atmosphere did not degas from the mantle. If correct and most volatiles remained at the surface, this would require that the atmosphere prior to and for some time after Moon-formation was massive enough to prevent significant erosion by impactors large and small.

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scattered outer Solar System planetesimals formed after ~3 Ma, they are likely to have been very volatilerich. This is the case for the CI, CM and CR carbonaceous chondrites as well as comets, and only relatively

# 14:40 - 15:00

## 52

# Stable isotopes - fingerprints for tracing the origin and history of building blocks and ingredients for life from molecular clouds to planets

Wampfler S<sup>1</sup>, Altwegg K<sup>2</sup>, Rubin M<sup>2</sup>, Haenni N<sup>2</sup>, Mueller D<sup>2</sup>, Jorgensen J<sup>3</sup>

<sup>1</sup>Center for Space and Habitability, University of Bern, <sup>2</sup>Physikalisches Institut, University of Bern, <sup>3</sup>Niels Bohr Institute, University of Copenhagen

Understanding the origin and evolution of the building blocks of planets and minor bodies, and eventually life, is challenging because of the complexity and long time scales involved in the star and planet formation process. Moreover, the most pristine materials in our own solar system, meteoritic inclusions and cometary ices, are present in the form of solids, whereas most of our information on the molecular composition of solar-like star-forming regions stems from observations of species in the gas-phase. Linking the solar system record to processes observed in nascent solar system analogues requires probes that can be used across a wide range of materials, in situ as well as by remote observations.

Stable isotope ratios of volatile elements such as D/H, <sup>14</sup>N/<sup>15</sup>N, <sup>16</sup>O/<sup>18</sup>O etc. can be measured in rocky, icy, and gaseous phases, and are therefore promising tracers for the origin and the evolution of volatiles and organic matter. However, using them as fingerprints for the history of planetary, cometary, and asteroidal building blocks and the delivery of volatiles requires a detailed understanding of the fractionation mechanisms and spatial and temporal evolution of the isotopic ratios during the formation of low-mass stars and their planetary systems.

In this contribution, we will present the current understanding of nitrogen isotopic fractionation in starforming regions, including new observational data investigating the presence of separate atomic and molecular nitrogen isotopic reservoirs with distinct compositions around young stars. We will also present in situ measurements of the <sup>14</sup>N/<sup>15</sup>N ratio by the Rosetta-ROSINA instrument at comet 67P, pointing at a single nitrogen isotopic reservoir in comets, in contrast to the results on protostars and protoplanetary disks. We will then conclude by explaining how a better understanding of the carrier phases of nitrogen may help in reconciling the cometary and interstellar pictures on nitrogen isotopes, and how these results can further contribute to developing the nitrogen isotopic ratio into a key signature for constraining the origin and evolution of different cosmomaterials from molecular clouds to planets.

# 15:00 - 15:20

### 991

# The molecular origin of life: interstellar prebiotic chemistry

### Niels F.W. Ligterink<sup>1</sup>

<sup>1</sup>Space Research & Planetary Sciences division, Physics Institute, University of Bern

The origin of life is intertwined with the emergence of complex organic molecules that act as the chemical building blocks of life. While prebiotic chemistry can take place on planets, for example in their atmospheres or in hydrothermal vents, a fascinating alternative is the production of prebiotic molecules in space.

In this talk, we will take a look at the prebiotic molecules we find in space. We use the ALMA radiotelescope to study the molecules in the gas around infant stars and planet-forming regions [1,2,3,4,5,6]. We find species that can act as building blocks of amino acids, sugars, peptides, and nucleobases. While these molecules are observed in the gas, evidence is found that they originally formed on microscopic ice-coated dust grains. In protoplanetary disks, these dust grains coaggulate together to form larger boulders, planetesimals, and eventually planets. Therefore, these interstellar prebiotic molecules can be inherited on planets, resulting in a rapid development of prebiotic chemistry and thus help kick-start the emergence of life.

[1] Ligterink, N. F. W., et al. "The ALMA-PILS survey: detection of CH3NCO towards the low-mass protostar IRAS 16293– 2422 and laboratory constraints on its formation." Monthly Notices of the Royal Astronomical Society 469.2 (2017): 2219-2229.

[2] Ligterink, Niels Frank Willem, et al. "The ALMA-PILS survey: Stringent limits on small amines and nitrogen-oxides towards IRAS 16293–2422B." Astronomy & Astrophysics 619 (2018): A28.

[3] Ligterink, N. F. W., et al. "The formation of peptide-like molecules on interstellar dust grains." Monthly Notices of the Royal Astronomical Society 480.3 (2018): 3628-3643.

[4] Ligterink, Niels FW, et al. "The family of amide molecules toward NGC 6334I." The Astrophysical Journal 901.1 (2020): 37.

[5] Ligterink, N. F. W., et al. "The prebiotic molecular inventory of Serpens SMM1-I. An investigation of the isomers CH3NCO and HOCH2CN." Astronomy & Astrophysics 647 (2021): A87.

[6] Ligterink, Niels FW, et al. "The prebiotic molecular inventory of Serpens SMM1: II. The building blocks of peptide chains." ACS Earth and Space Chemistry 6.3 (2022): 455-467.

# 15:20 - 15:40

# 18

# Tracing Volatiles from Protoplanetary Disks to Planetary Atmospheres

### Wang H<sup>1</sup>, Mordasini C<sup>2</sup>, Drążkowska J<sup>3</sup>, Quanz S<sup>1</sup>

<sup>1</sup>ETH Zurich, Institute for Particle Physics and Astrophysics, <sup>2</sup>Physikalisches Institut, Universität Bern, <sup>3</sup>University Observatory, Faculty of Physics, Ludwig-Maximilians-Universität München

The bulk composition of a planet-hosting star is thought to reflect the initial chemical composition of the protoplanetary disk from which planets form. However, deviations in the composition of (particularly rocky) planets from their host star are commonplace, and may occur by gas-dust fractionation in the protoplanetary disk and/or over the dynamical process of planet formation. A key distinguishing feature between the formation of a gas giant (e.g. Jupiter) and a rocky planet (e.g. Earth) is devolatilization, i.e., depletion of volatiles, which include both atmophiles (e.g. H, C, N and noble gases) and moderately volatile minerophiles (e.g. O, S, Si, Mg and Fe). This devolatilization mechanism has been observed empirically both in the Solar System and in other planetary systems (e.g. in the atmospheres of polluted white dwarfs), but has yet to be accounted for in most (if not all) existing models of planet formation.

Here, we present a comprehensive interpretation of both nebular (e.g. dust formation, condensation, and evaporation/sublimation) and post-nebular (e.g. energetic accretion and impacts, hydrodynamic escape, and photoevaporation) devolatilization processes as well as our research scheme of incorporating these processes into state-of-the-art planet formation models. Based on our previous empirical studies of these processes, the importance of devolatilized host stellar abundances, along with measured planetary masses and radii, will be demonstrated in constraining the detailed properties of rocky exoplanets including both interiors and atmospheres. Ultimately, by tracing the evolutionary path of both life-critical and rock-essential volatiles (e.g. H, C, O, N, S, Mg, Si and Fe) during planet formation and evolution, this will help us understand why and how our planet becomes habitable and inhabited, and the extent to which we can make testable predications about the habitable conditions of rocky exoplanets apt for life emergence and prevalence in the cosmos.

# 39

# Solubility of water in peridotite liquids and the prevalence of steam atmospheres on rocky planets

Sossi P<sup>1</sup>, Tollan P<sup>1</sup>, Badro J<sup>2</sup>, Bower D<sup>3</sup>

<sup>1</sup>ETH Zürich, <sup>2</sup>Institut de Physique du Globe de Paris, <sup>3</sup>Universität Bern

Atmospheres are products of time-integrated mass exchange between the surface of a planet and its interior. On Earth and other planetary bodies, magma oceans likely marked significant atmosphere-forming events, during which both steam- and carbon-rich atmospheres may have been generated. However, the nature of Earth's early atmosphere, and those around other rocky planets, remains unclear for lack of constraints on the solubility of water in liquids of appropriate composition. Here we determine the solubility of water in 14 peridotite liquids, representative of Earth's mantle, synthesised in a laser-heated aerodynamic levitation furnace. We explore oxygen fugacities (fO2) between -1.9 and +6.0 log units relative to the iron-wüstite buffer at constant temperature (1900±50 °C) and total pressure (1 bar). The resulting fH2O ranged from nominally 0 to 0.027 bar and fH2 from 0 to 0.064 bar. Total H2O contents were determined by transmission FTIR spectroscopy of doubly-polished thick sections from the intensity of the absorption band at 3550 cm-1 and applying the Beer-Lambert law. The mole fraction of water in the liquid is found to be proportional to (fH2O)0.5, attesting to its dissolution as OH. The data are fitted by a solubility coefficient of ~525 ppm/bar0.5, roughly 25 % lower than for basaltic liquids at 1350 °C and 1 bar. Higher temperatures (rather than more magnesian compositions) result in a significant decrease of water solubility in silicate melts. Because the solubility of water remains high relative to that of CO2, steam atmospheres are rare, although they may form under moderately oxidising conditions on telluric bodies, provided sufficiently high H/C ratios prevail.

# 16:35 – 16:55

# 10

# Interstellar origins of chemical complexity in comets

### Drozdovskaya M<sup>1</sup>

<sup>1</sup>Center for Space and Habitability (CSH), Universität Bern

It has been speculated that chemically complex molecules could have been delivered to Earth during the Late Heavy Bombardment for further synthesis of biotic compounds on the planet. In my contribution, I will demonstrate the interstellar origins of cometary molecules. I will suggest that the large complex organic reservoirs in comets make them strong candidates for sowing the initial seeds of life on the early Earth. The earliest stage of star formation, the prestellar core, is the birth place of complex organic molecules under interstellar physical conditions. Upon gravitational collapse, a young protostar with a protoplanetary disk is formed. The concurrent heating and UV irradiation boost the production of complex organics. It is thought that the largest reservoir of complex organics is in interstellar ices. Desorption in the warm inner regions around protostars allows us to readily observe these species in the gas. In the outer parts of a protoplanetary disk, solid complex organics become integrated into cometesimals. I will highlight recent observational investigations of complex organics from cores to protostars, including studies of methanol isotopologs in the prestellar core L1544 (Kulterer et al. in prep.) and the comprehensive chemical inventory of the low-mass star-forming region IRAS 16293-2422 (e.g., Jorgensen et al. 2018; Drozdovskaya et al. 2018, 2022). I will bring forward the idea that comets of our Solar System reflect to a degree the complex organic composition of the innate core that birthed our Sun (Drozdovskaya et al. 2019, 2021).

# 16:55 – 17:15

# 27

# Geophysical and cosmochemical evidence for a volatile-rich Mars

**Khan A<sup>1</sup>**, Sossi P<sup>1</sup>, Liebske C<sup>1</sup>, Giardini D<sup>1</sup>, Rivoldini A<sup>2</sup> <sup>1</sup>*ETH Zurich,* <sup>2</sup>*Royal Observatory of Belgium* 

Constraints on the composition of Mars principally derive from chemical analyses of a set of Martian meteorites that rely either on determinations of their refractory element abundances or isotopic compositions. Both approaches, however, lead to models of Mars that are unable to self-consistently explain major element chemistry and match its observed geophysical properties, unless ad hoc adjustments to key parameters, namely, bulk Fe/Si ratio, core composition, and/or core size are made. Here, we combine geophysical observations, including high-quality seismic data acquired with the InSight mission, with a cosmochemical model to constrain the composition of Mars.

We employ the InSight seismic data, including a set of geophysical observations (tidal response, mean planetary density and moment of inertia) that sense the large-scale structure of Mars, to determine mantle and core composition. For this, we rely on a geophysical parameterization that provides a unified description of mantle and core phase equilibria and physical properties as a function of composition, temperature, and pressure. Based on the geophysically-determined mantle compositions and mean core properties (radius and density), we further employ a cosmochemical approach by focusing on major elements and the extant correlation between Fe/Si and Fe/Mg that is observed in planetary materials. Quantitative comparison of the geophysical and cosmochemical compositions enables us to restrict the mantle composition of Mars by considering only those compositions that fit both constraints. Finally, we employ the jointly-predicted mantle composition to place constraints on the identities and abundances of light elements in the Martian core. The novelty of our approach lies in the inversion of multiple geophysical observations to derive physically-credible solutions of the interior state of Mars, in conjunction with cosmochemically-plausible bulk chemical compositions.

We find that: 1) mantle FeO content varies in the range 12.5–15 wt%, which is several wt% lower than suggested by canonical models that derive from geochemical analyses of Martian meteorites; 2) a lower mantle FeO content generally correlates with a lower MgO and higher SiO2 content. The radius range of the liquid core found here is 1790–1870 km and the core density range is 6-6.3 g/m3, as a consequence of the lower mantle FeO content of the mantle. The core compositions most compatible with these numbers, based on thermodynamic solution models constructed from experimental data, are found to encompass 9 wt% S,  $\geq$ 3 wt% C,  $\leq$ 2.5 wt% O, and  $\leq$ 0.5 wt% H, supporting the notion of a volatile-rich Mars. To accumulate sufficient amounts of these volatile elements, Mars must have formed before the nebular gas dispersed and/or, relative to Earth, accreted a higher proportion of planetesimals from the outer proto-planetary disk where volatiles condensed more readily.

# 17:15 – 17:35

# 14

# Life under fire: collisional evolution of the prebiotic Earth

**Walton C**, Wyatt M, Anand M, Cernok A, Suttle M, Shorttle O <sup>1</sup>University Of Cambridge

The Earth likely experienced a greater rate of collisions with extraterrestrial matter in early Solar System history. This is highly relevant for the chemical origins of life, as many types of extraterrestrial matter are enriched in life-limiting elements relative to Earth's crust. I will present results from a continuing effort to interrogate (i) collisional activity in the early Solar System, (ii) the implications of that collisional history for accretion of life-limiting elements to the surface of prebiotic Earth, and (iii) the surface processing of extraterrestrial matter in the context of origin of life chemistry. These topics in turn are investigated with isotopic analyses of meteorites from asteroids that experienced collisions, geochemical measurements of the fine-grained cosmic dust particles that those collisions generated, and simulations of extraterrestrial matter processing and ensuing prebiotic chemistry in closed-basins on prebiotic Earth. Our combined approach leverages astrophysical, geological, and chemical constraints to better understand the role and relevance of collisional bombardment in seeding planets for life.

# Day 2, Wednesday, 31.8.2022

# Table of Content: Session 2 Talks

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**60** Volcanic activity and formation of the continental crust in the early earth **Bachmann O<sup>1</sup>**, Laurent O<sup>2</sup>, Moyen J<sup>3</sup>, Ulmer P<sup>1</sup>, Wotzlaw J<sup>4</sup> <sup>1</sup>Ethz, <sup>2</sup>CNRS; Géosciences Environnement, <sup>3</sup>Université Jean Monnet, <sup>4</sup>Accelopment

**46** Atmospheric Nitriles for the Origin of Life after Large Asteroid Impacts on the Hadean Earth **Wogan N<sup>1</sup>**, Catling D<sup>1</sup>, Zahnle K<sup>2</sup> <sup>1</sup>University Of Washington, <sup>2</sup>NASA Ames

**71** Study of habitability of Archean Earth with Earth-like planet Surface Temperature Model (ESTM) Ivanovski S<sup>1,2</sup>, Surtchev Y<sup>1</sup>, Bevilacqua R<sup>2</sup>, Vladilo G<sup>1</sup>, Silva L<sup>1,3</sup>, Simonetti P<sup>1,2</sup>, Biasiotti L<sup>1,2</sup>, Bisesi E<sup>1</sup>, Maris M<sup>1,3</sup>, Murante G<sup>1,3</sup> <sup>1</sup>Astronomical Observatory of Trieste, <sup>2</sup>UniTs, <sup>3</sup>IFPU

**44** Micropyrite: a promising biosignature? Insights from modern and ancient sediments Marin Carbonne J<sup>1</sup>, Decraene M<sup>1</sup>, Dupeyron J<sup>1</sup>, Alléon J<sup>1</sup>, Olivier N<sup>2</sup>, Thomazo C<sup>3</sup>, Bernard S<sup>4</sup> <sup>1</sup>University Of Lausanne, <sup>2</sup>Université Clermont Auvergne, <sup>3</sup>Université Bourgogne Franche Comté, <sup>4</sup>Sorbonne Université

# Poster

**66** Lagrangian points as the origin of giant impactors Balsalobre-Ruza O<sup>1</sup>, Lillo-Box J<sup>1</sup>, Huélamo N<sup>1</sup>, López-Ibáñez L<sup>2</sup> <sup>1</sup>Center for Astrobiology (CAB), <sup>2</sup>Complutense University of Madrid (UCM)

# 9:00 - 9:40

### **KEYNOTE**

## Environmental conditions for the origin of life and the spread of early life.

#### David Catling<sup>1</sup>

<sup>1</sup>University of Washington

I will review advances in our understanding of the co-evolution of life and environment on the Earth from about 4.5 billion years ago to the rise of atmospheric oxygen beginning around 2.4 billion years ago. I will argue that the expected chemical composition of the early atmosphere and surface waters favored prebiotic syntheses and the origin of life. By the Archean eon (4 to 2.5 billion years ago), the geologic record increasingly holds clues to the nature of the atmosphere and biosphere, which are reflected in isotope systems, the composition of marine and non-marine sediments, and occasionally physical aspects of rocks. I will conclude that understanding the young Earth is necessary in the search for biosignatures elsewhere because analogous stages of early evolution arguably occur on other rocky worlds.

# 9:40 - 10:00

### 60

# Volcanic activity and formation of the continental crust in the early earth

**Bachmann O<sup>1</sup>**, Laurent O<sup>2</sup>, Moyen J<sup>3</sup>, Ulmer P<sup>1</sup>, Wotzlaw J<sup>4</sup> <sup>1</sup>Ethz, <sup>2</sup>CNRS; Géosciences Environnement, <sup>3</sup>Université Jean Monnet, <sup>4</sup>Accelopment

Granitoids of the tonalite-trondhjemite-granodiorite (TTG) series dominate Earth's earliest continental crust. The geochemical diversity of TTGs is ascribed to several possible geodynamic settings of magma formation, from low-pressure differentiation of oceanic plateaus to high-pressure melting of mafic crust at convergent plate margins. These interpretations implicitly assume that the bulk-rock compositions of TTGs did not change from magma generation in the source to complete crystallization. However, crystal-liquid segregation influences the geochemistry of felsic magmas, as shown by the textural and chemical complementarity between coeval plutons and silicic volcanic rocks in the Phanerozoic Eon. We demonstrate here that Paleoarchean (ca. 3,456 million years old) TTG plutons from South Africa do not represent liquids but fossil, crystal-rich magma reservoirs left behind by the eruption of silicic volcanic rocks, being possibly coeval at the million-year scale as constrained by high-precision uranium-lead geochronology. The chemical signature of the dominant trondhjemites, conventionally interpreted as melts generated by high-pressure melting of basalts, reflects the combined accumulation of plagioclase phenocrysts and loss of interstitial liquid that erupted as silicic volcanic rocks. Our results indicate that the entire compositional diversity of TTGs could derive from the upper crustal differentiation of a single, tonalitic magma formed by basalt melting and/or crystallization at <40!km depth. These results call for a unifying model of Hadean–Archean continent nucleation by intracrustal production of TTG magmas, and highlight the importance of silicic volcanism in the early earth.

## 46

# Atmospheric Nitriles for the Origin of Life after Large Asteroid Impacts on the Hadean Earth

**Wogan N<sup>1</sup>**, Catling D<sup>1</sup>, Zahnle K<sup>2</sup> <sup>1</sup>University Of Washington, <sup>2</sup>NASA Ames

While there are several theories for the origin of life, the presence of nucleotide "fossils" in modern biology has led to the RNA World hypothesis. This hypothesis proposes a stage of primitive life with RNA as a catalyst and as a self-replicating molecule that evolved by natural selection, which, at some point, was encapsulated in a cell. RNA needs to be produced abiotically on early Earth in this scenario. Chemists have demonstrated several schemes in the lab, but all pathways require nitriles – hydrogen cyanide (HCN), cyanoacetylene (HCCCN), and cyanogen (NCCN) – to synthesize the nucleobases of RNA.

Abiotic synthesis of nitriles very likely requires a reducing prebiotic atmosphere, i.e., one redox-dominated by hydrogen-bearing reducing gases, and consisting of, e.g., H2, CH4 with CO2 or CO, and N2 and/or NH3. Photochemistry makes HCN from the nitrogenous gases only if CH4 is abundant. Also, HCCCN and NCCN are produced in highly reducing atmospheres, e.g. Titan's.

However, geochemical evidence suggests that volcanoes did not produce very reduced gases in the Hadean, and abundant volcanic CH4, in particular, was unlikely. Instead, impacts are a plausible source.

Asteroid impacts would make a reducing atmosphere because reactions between iron-rich impact ejecta and shock-heated water vapor from the ocean would generate substantial amounts of H2, CH4 and possibly NH3. Subsequent photochemistry would have generated prebiotic molecules like HCN making a "window of opportunity" for abiotic synthesis and evolution of RNA.

We simulated creation and evolution of impact-generated reducing atmospheres with a novel 1dimensional photochemical model, improving upon previous work (1). We quantified the surface deposition of atmospheric nitriles following impacts with impactor diameters between 300 and 2000 km. We also used a 1-dimensional climate model to estimate the surface temperature of these hydrogen-rich atmospheres to examine the fate of nitriles at Earth's surface.

1. Zahnle, Lupu, Catling & Wogan (2020). Creation and evolution of impact-generated reduced atmospheres of early Earth. Planetary Science Journal. doi:10.3847/PSJ/ab7e2c.

# 71

# Study of habitability of Archean Earth with Earth-like planet Surface Temperature Model (ESTM)

**Ivanovski S<sup>1,2</sup>**, Surtchev Y<sup>1</sup>, Bevilacqua R<sup>2</sup>, Vladilo G<sup>1</sup>, Silva L<sup>1,3</sup>, Simonetti P<sup>1,2</sup>, Biasiotti L<sup>1,2</sup>, Bisesi E<sup>1</sup>, Maris M<sup>1,3</sup>, Murante G<sup>1,3</sup>

<sup>1</sup>Astronomical Observatory of Trieste, <sup>2</sup>UniTs, <sup>3</sup>IFPU

The question of the existence of extraterrestrial life has been a long-standing aspiration of humanity. Studying the physical, geological, and chemical conditions of exoplanets will advance our understanding of their potential to host life. Our concept of life is based on the life found on Earth. First, we study young Earth as an aqua planet, received energy from a fainter Sun, and had thousands of times more atmospheric CO2, and no oxygen. One of the most important quantities to consider for habitability is temperature. We have performed simulations with an Earth-like planet Surface Temperature Model (ESTM, Vladilo et al. 2015; Biasiotti et al. 2022) to study the habitability of Archean Earth. Sun luminosity and the Earth rotational period between 2.5 and 4 billion years ago were used as input parameters. Two other key parameters were varied: ocean fraction and atmospheric content of CO2. We found that too much CO2 resulted in a blistering hot planet even in the conditions of a faint Sun. Ocean fraction was essential for habitability since our simulations demonstrated that a very dry planet and a moderate amount of CO2, would turn the planet into a snowball. But if there is an abundance of CO2, even a small amount of water would be sufficient to make an Earth-like planet habitable.

We review the recent advances in the modelling of habitability as a function of various hosting star parameters and planetary evolution characteristics using an ESTM model developed at the Astronomical Observatory of Trieste.

References

Biasiotti, L., et al., 2022, MNRAS Vladilo, G., et al., 2015, ApJ, 804, 50

## 11:20 - 11:40

### 44

Micropyrite: a promising biosignature? Insights from modern and ancient sediments

**Marin Carbonne J<sup>1</sup>**, Decraene M<sup>1</sup>, Dupeyron J<sup>1</sup>, Alléon J<sup>1</sup>, Olivier N<sup>2</sup>, Thomazo C<sup>3</sup>, Bernard S<sup>4</sup> <sup>1</sup>University Of Lausanne, <sup>2</sup>Université Clermont Auvergne, <sup>3</sup>Université Bourgogne Franche Comté, <sup>4</sup>Sorbonne Université

Identifying (micro)fossils from the Earth's early biosphere is ambitious and challenging due to the scarcity of the oldest rocks and their complex post depositional history. The first form of life was small, like microorganisms, and produce ambiguous fossil forms and chemical and isotopic signatures, which are not unique. Therefore, almost all early life trace discoveries have been strongly discussed and disputed. Here, we propose that pyrite, an iron sulfide, ubiquitous in sedimentary rocks, is a promising biosignature. Indeed, in modern environments, pyrite is a by-product of various metabolic activities, such as microbial sulfate reduction and iron dissimilatory reduction. We will present detailed mineralogical and isotope studies of ancient and modern sediments that highlight the potential of micropyrites to capture (and retain) microbial signatures through time. We have developed an original approach, combining high resolution microscopy with S and Fe isotopes characterization at a micrometer scale using SIMS and NanoSIMS analyses . We will show that studied micropyrites record the oldest signature of dissimilatory iron reduction and microbial sulfate reduction, which suggest the presence of diversified microbial biocoenoses during the (Paleo)Archean.

## Poster

### 66

# Lagrangian points as the origin of giant impactors

**Balsalobre-Ruza O<sup>1</sup>**, Lillo-Box J<sup>1</sup>, Huélamo N<sup>1</sup>, López-Ibáñez L<sup>2</sup> <sup>1</sup>Center for Astrobiology (CAB), <sup>2</sup>Complutense University of Madrid (UCM)

The role of giant impacts in the construction of habitable worlds is known to be a key piece of the Astrobiology puzzle not yet fully explored. These impacts between large bodies during the formation and early stages of planetary systems are known to occur with relatively high frequency. Some of their consequences are the mix-up of materials between the two bodies, the extraction of processed material from the interior of the forming planets or the depletion and replenishment of the planetary atmosphere. Another consequence is the potential formation of natural satellites, known to have an important role in the life sustainability in our own Earth-Moon system. But, where do these bullets come from? Their origin is key to understand the available and deposited material that is then at the disposal for abiogenesis. One of the possible origins of these impactors are the so-called Lagrangian points. In this poster we explore this possibility in the context of the TROY project and the search for co-orbital exoplanets.

# Day 2 & 3, Wednesday, 31.8. & Thursday, 1.9.2022

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# Session 3

# Talks

### **KEYNOTE**

# Dew RNA world: starting evolution from the solid state

### Dieter Braun1

<sup>1</sup>LMU München

Understanding the emergence of life means to recreate a physico-chemical system that is capable of open ended Darwinian evolution. The more simple it is and the less special compounds and conditions it require, the more probably it can occur. We will discuss experiments that imply a fundamentally simplified RNA world that starts from the solid state.

We revisited polymerization and templated ligation of RNA from nucleotides with 2',3' cyclic phosphates. They oligomerized under alkaline conditions at pH 9-11 without catalysts or added salts, reaching 10 mers in a day, both in the 'dry' state or in the wet-dry cycling at a heated air-water interface [1]. At high temperatures, the oligomers were dominated by G, but cold and dry conditions, achieved in the planet simulator of McMaster University, yielded random sequences of GC or GCAU. The yield for oligonucleotides which contain still a functional 2'3'-phosphate peaks between 4°C and 25°C.

Under similar conditions, phosphorylation from Trimetaphosphate and templated ligation was observed under such "dry" conditions. We envisage therefore a one pot reaction from nucleosides to the replication of oligomers. The separation of strands would be provided by the condensation of salt-free dew droplets which also dissolve new feeding nucleosides from the solid state, triggering another cycle of phosphorylation, polymerization and templated ligation in the "dry" state. A likely driving for this mechanism would be the day night cycles. We are searching for short RNA sequences to enhance this replication by ligation in the dry state, leading to a much simplified RNA world to trigger self-amplified biological evolution of functional sequences.

In deeper layers of the porous rock, we envisage that air-water interfaces drive more sophisticated Ribozymes. We shown that CO2-water interfaces can drive the replication towards sequence lengths of up to 1300 mers, overcoming the tyranny of the shortest by the length selective accumulation under evaporation-based capillary flow. The long strands separate under the pH and salt cycling provided by the Hadean atmosphere of CO2. While the replication was still implemented by a polymerase to enhance kinetics, preliminary results show a similar strand separation for Ribozymes under elevated Mg2+ concentrations.

[1] doi:10.26434/chemrxiv-2022-zwh2t (2022)

[2] Nature Physics doi.org/10.1038/s41567-022-01516-z (2022)

# 14:10 - 14:30

### 11

# Prebiotic chemistry networks for carbon fixation and joining building blocks

Liu Z<sup>1</sup>

### <sup>1</sup>MRC - Laboratory Of Molecular Biology

Life is an out-of-equilibrium system sustained by a continuous supply of energy. In extant biology, the generation of the primary energy currency, adenosine 5'-triphosphate and its use in the synthesis of biomolecules require enzymes. Before their emergence, alternative energy sources, perhaps assisted by simple catalysts, must have mediated the prebiotic chemistry reactions. Here I will present two examples for these prebiotic chemistry reaction networks. Firstly, we demonstrate an efficient ultraviolet photoredox chemistry between CO2 and sulfite that generates organics and sulfate. The chemistry is initiated by electron photodetachment from sulfite to give sulfite radicals and hydrated electrons, which reduce CO2 to its radical anion. A network of reactions that generates citrate, malate, succinate and tartrate by irradiation of glycolate in the presence of sulfite was also revealed. The simplicity of this carboxysulfitic chemistry and the widespread occurrence and abundance of its feedstocks suggest that it could have readily taken place on the surfaces of rocky planets. The availability of the carboxylate products on early Earth could have driven the development of central carbon metabolism before the advent of biological CO2 fixation. Secondly, I will talk about that the chemical energy inherent to isonitriles can be harnessed to activate nucleoside phosphates and carboxylic acids through catalysis by acid and 4,5-dicyanoimidazole under mild aqueous conditions. Simultaneous activation of carboxylates and phosphates provides multiple pathways for the generation of reactive intermediates, including mixed carboxylic acid-phosphoric acid anhydrides, for the synthesis of peptidyl–RNAs, peptides, RNA oligomers and primordial phospholipids.

## 20

# Heterogeneous Reactants at the Origin of Life: Towards Prebiotically Plausible Nonenzymatic RNA Copying

**Duzdevich D<sup>1</sup>**, Carr C<sup>2</sup>, Zhang S<sup>1</sup>, Szostak J<sup>1</sup> <sup>1</sup>Harvard University, <sup>2</sup>Georgia Institute of Technology

The RNA World hypothesis posits that RNA played an essential role during the origin of life by serving as both the hereditary material, and the primary molecule of function in the form of ribozymes. The Szostak laboratory uses model systems to experimentally study how primitive forms of RNA propagation may have emerged in the absence of enzymes. A key step on the pathway to achieving nonenzymatic RNA replication is nonenzymatic template-directed nucleotide polymerization. Experiments in this field typically employ defined or homogenous template sequences and one or only a few chemically activated nucleotide species (for example, a poly-rG template and rC reactants). A more realistic scenario is to consider random templates and all four canonical nucleotide reactants. We recently developed a sequencing assay that has enabled us to characterize this scenario for the first time. We were especially interested in understanding the origin of mismatches, which are much more common without the work of enzymatic regulation, and found that correct copying in our system depends on the prevalence of a previously-identified 5'-5' bridged dinucleotide reactant.

We are adapting this assay to consider progressively more realistic scenarios. First, we have incorporated a prebiotically plausible methyl isocyanide-based nucleotide activation chemistry (instead of using artificially-activated and purified reactants). This approach improves reaction fidelity because the activation chemistry drives the formation of the bridged dinucleotide, thereby increasing the probability of correct incorporations. Second, we are introducing greater heterogeneity among reactants by including various sets of short oligonucleotides. Previous work with defined sequences has shown that oligos can facilitate copying, but here we consider whether those improvements apply in a random-sequence context, and also whether the oligos benefit copying fidelity. Preliminary results suggest that these more realistic conditions can improve nonenzymatic copying, indicating that future work should embrace the heterogenous conditions that would have prevailed during the emergence of life.

# 14:50 - 15:10

### 990

# An analysis of nucleotide-amyloid interactions reveals binding to codonsized RNA

Saroj K. Rout, Anna Knörlein, Jonathan Hall, Jason Greenwald and Roland Riek

### <sup>1</sup>ETH Zurich

Interactions between RNA and proteins are the cornerstone of many important biological processes from transcription and translation to gene regulation, yet little is known about the ancient origin of said interactions. We have hypothesized that peptide amyloids played a role in the origin of life and that their repetitive structure lends itself to building interfaces with other polymers through avidity. Here we report that short RNA with a minimum length of three nucleotides bind in a sequence-dependent manner to peptide amyloids. The 3'-5' linked RNA backbone appears to be well-suited to support these interactions with the phosphodiester backbone and nucleobases both contributing to the affinity. Sequence specific RNA-peptide interactions of the kind identified here may provide a path to understanding one of the great mysteries rooted in the origin of life: the origin of the genetic code.

# 15:45 – 16:05

## 34

# Photochemical Reactions in Lakes on Early Earth

**Kufner C<sup>1</sup>**, Lozano G<sup>1</sup>, Mast C<sup>2</sup>, Zinth W<sup>2</sup>, Braun D<sup>2</sup>, Ranjan S<sup>3</sup>, Todd Z<sup>4</sup>, Sasselov D<sup>1</sup> <sup>1</sup>Harvard University, <sup>2</sup>Ludwig-Maximilians-University, <sup>3</sup>Northwestern University, <sup>4</sup>University of Washington

On the surface of the Early Earth, ultraviolet (UV) light is a key energy source for the formation of the building blocks of life.[1] However, it has remained an open question how deep UV light could have penetrated into natural waters on Early Earth or comparable exoplanetary systems. We studied the UV absorption spectra of a variety of salts available on Early Earth in the prebiotically abundant wavelength range between 200 nm to 360 nm.[2] As a result, we found wavelength dependent penetration depth. For all salts studied, we obtained low penetration depths for wavelengths around 200 nm and deeper penetration for longer wavelengths. Depending on their wavelength, the photons in the ultraviolet range between 200 nm and 360 nm can trigger a variety of photochemical reactions in prebiotic molecules: The absorption of a photon below 250 nm can eject solvated electrons from sulfite into the solution which have been shown to be essential to trigger reductive photochemistry[3] underneath the surface of prebiotic lakes. Photons with wavelengths up to 290 nm can induce sequence selective processes on short nucleic acids at higher depths. Nucleic acids strands can be destroyed photochemically in a sequence-dependent manner, yielding a selection of early sequences which could have formed the first proto-genomes. We determined the 266 nm UV stability of short DNA single strands, which consist of a random sequence of 8 bases in a massively parallel approach by next-generation sequencing.[4] Our findings strongly indicate that the UV stability of sequences could have influenced the development of codon/anticodon pairs in the evolution of life.

a) M. W. Powner, B. Gerland, J. D. Sutherland, Nature 2009, 459, 239–242; b) J. Xu, N. J. Green, D. A. Russell, Z. Liu, J. D. Sutherland, J. Am. Chem. Soc. 2021, 143, 14482-14486; c) S. Ranjan, R. Wordsworth, D. D. Sasselov, The Astrophysical Journal 2017, 843, 110.

[2] S. Ranjan, C. L. Kufner, G. G. Lozano, Z. R. Todd, A. Haseki, D. D. Sasselov, Astrobiology 2022, 22, 242-262.

[3] Z. Liu, L.-F. Wu, C. L. Kufner, D. D. Sasselov, W. W. Fischer, J. D. Sutherland, Nature Chemistry 2021, 13, 1126-1132.

[4] C. L. Kufner, S. Krebs, M. Fischaleck, J. Philippou-Massier, H. Blum, D. B. Bucher, D. Braun, W. Zinth, C. B. Mast, Manuscript in preparation 2022.

# 16:05 - 16:24

### 36

# Impact of radioactive potassium on the emergent molecular structures of terrestrial life

### Vladilo G<sup>1</sup>

<sup>1</sup>INAF - Osservatorio Astronomico di Trieste

Natural radionuclides are often considered as potential actors in the general scenario of prebiotic chemistry. Most of the studies driven by this idea have examined the radiochemical impact induced by the unstable isotopes of uranium and thorium. These heavy isotopes could play a role in the early prebiotic stages, but their decay products (alpha particles and unstable nuclei) would severely damage the key molecular structures that are expected to emerge at later stages (e.g., replicating and/or catalytic molecules). In this presentation I will examine a different radionuclide, the potassium isotope 40K, and its decay products (mostly beta particles and stable nuclei) that have a milder radiochemical impact. Potassium is abundant and widespread in the Earth crust and oceans, whereas uranium and thorium are rare and concentrated in specific niches. Therefore, potassium (including its unstable isotope) was likely to be present in prebiotic chemistry, starting from the very earliest stages. Moreover, assuming continuity with extant biology, potassium (including its unstable isotope) was probably incorporated in the earliest, fully developed terrestrial cells. Based on these arguments, 40K was likely to be present in all the prebiotic stages and, with a proper flux of decaying particles, may have influenced the molecular evolution leading to the emergence of life. The fact that the isotopic ratio 40K/K was one order of magnitude higher than today when terrestrial life was born (early Archean) supports this possibility. For plausible values of potassium concentration, the specific rate of 40K decays in an Archean aqueous medium could have been two orders of magnitude higher than in present-day eukaryotic cells. Preliminary estimates of the potential prebiotic impact of the resulting flux of beta particles will be provided in my talk. Molecular structures may be affected depending on: (i) the possibility of accumulating radiochemical effects and (ii) the distance range over which the cooperation of intermolecular forces can propagate the effects of beta decays. In the final part of my presentation I will discuss a further reason for examining the case of 40K, related to the origin of the homochirality of biological biomolecules. The potential link between homochirality and 40K is the parity violation of the beta decay, as a result of which the spin component of the emitted fast electrons is always antiparallel to the direction of motion. By coupling their spin with that of the molecules encountered along their path, the beta particles may induce a chiral imprint in the molecular structures. Despite the large number of studies trying to link the origin of homochirality to physical processes, the effects of a persistent injection of beta particles in protobiological structures have never been examined. The origin of homochirality is an open question in studies of abiogenesis and the possible impact of 40K decays in this context should be quantified. Future steps to be undertaken for casting light on this subject will be briefly summarized.

# 16:25 – 16:45

### 42

### Meteorite Impacts and the Emergence of Life

**Sapers H<sup>1</sup>**, Cockell C<sup>3</sup>, Osinski G<sup>2</sup>, Pontefract A<sup>2</sup> <sup>1</sup>York University, <sup>2</sup>The University of Western Ontario, <sup>3</sup>University of Edinburgh

Impact structures on Earth are often overlooked from a biological perspective even though they are a fundamental process in planetary evolution – indeed – they are the most common geological feature in the Solar System. The increased frequency of large impacts early in the Earth's history, commensurate with the origin and early evolution of life, has led to two hypotheses: 1) impact events frustrated the emergence of life, and 2) the energy and geochemical products of impact events facilitated habitability. Proposing a paradigm shift from sporadic, biologically destructive events, we posit that periods of high impact flux early in planetary evolution drive planetary habitability and facilitate the emergence of life. The impact creating process both generates the conditions conducive to the origin of life as well as creates varied habitats for life that persist for thousands to millions of years following the impact event. Impact cratering generates subaerial and submarine hydrothermal systems in varied geochemical settings resulting in a diverse suite of water-rock reactions including serpentinization. Shock-metamorphism during an impact event results in unique geological materials such as impact analogues for volcanic pumice rafts in splash pools that provide protective niches and vesicular voids lined with phyllosilicate minerals and other catalytic substrates allowing for the concentration of pre-biotic chemicals. The impact process itself delivers many of the ingredients thought to be important in the early development of planetary habitability and the emergence of life such as complex organics and the atmospheric generation of hydrogen cyanide. Transient impactassociated hydrological systems, and the geological products of shock metamorphism such as impact glass and shocked crystalline rock that provide unique endolithic and lithotrophic niches persist long after impact. This work does not contradict existing environments proposed for the origin of life on Earth, rather we present the impact crater and the crating process as an alternative mechanism to create the previously proposed environments and conditions necessary for the emergence of life. The impact process does not rely on other active geological processes such as plate tectonics, or volcanism and as such, impact cratering is ubiquitous on rocky and icy bodies in the Solar System, independent of size, internal heating mechanisms, and distance from the Sun. Impact events therefore potentially represent a mechanism to generate habitability on other planets, satellites, and even asteroids throughout and beyond the Solar System with implications for not only understanding the emergence of life on Earth, but a parsimonious mechanism for the putative emergence of life on other rocky and icy bodies. The most striking example of impactassociated biospheres on Earth are in the subsurface. Arguably, the most compelling environment in which to search for life beyond Earth is in the subsurface of other potentially habitable Solar System bodies such as Mars. Impact structures thus comprise novel modern subsurface environments that provide unique opportunities to study extant subsurface life on Earth with implications in the development of planetary habitability and for the emergence of life on Earth and potential for life elsewhere in the Solar System.

# 1.9.2022

8:45 - 9:05

49

# Formation rates of ferrocyanide on the early Earth and their implications for prebiotic chemistry

**Todd Z<sup>1</sup>**, Catling D<sup>1</sup> <sup>1</sup>University Of Washington

Ferrocyanide, a potentially important compound for the origins of life, could have been present on the early Earth in various geochemical environments. In addition to being an important prebiotic ingredient itself (e.g. Xu et al. 2018), ferrocyanide could provide a mechanism for storing and stockpiling other prebiotic molecules, including cyanide (Sasselov et al. 2020). While previous studies have examined the conditions under which ferrocyanide formation is thermodynamically favored (Toner and Catling 2019), the kinetics of ferrocyanide formation remain an open question.

Here, we investigate the rate of formation and formation efficiency of ferrocyanide from solutions containing various concentrations of ferrous iron and hydrogen cyanide, under a range of pHs. We find that this reaction occurs on fairly short timescales, reaching completion on the order of minutes to hours. We further find that formation efficiency is significantly increased at more basic pHs.

The results have implications for understanding what concentrations of ferrocyanide are plausible, and furthermore, what timescales are relevant for ferrocyanide formation on the early Earth. By quantifying the rate of this reaction, we can further build up a model of prebiotic lake chemistry and determine implications for prebiotic chemistry on the early Earth. Given the potential importance of ferrocyanide as a source of stockpiling the prebiotically relevant molecule cyanide, these results are significant for understanding the robustness of prebiotic lake chemistry invoked under early Earth conditions.

References:

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## 54

# Non-enzymatic templated ligation of oligonucleotides containing 2',3' cyclic phosphate

Wunnava Venkata S<sup>1</sup>, Serrão A <sup>1</sup>LMU Munich CeNS

Replication of genetic information is a necessary step for the emergence of life. Recently, we showed that 2',3'- cyclic nucleotides can polymerize non-enzymatically under alkaline drying conditions. In the current work, we expand on that work to show that oligonucleotides with 2',3'-cyclic phosphate end can ligate on a complementary template. The reaction proceeds in alkaline pH 9-11 aqueous solutions with 1mM MgCl2 at 25 °C. Under the optimum conditions the reaction yields ~ 20% of product at 24h at pH 10 and is possibly only limited by the hydrolysis of the 2'3' cyclic phosphate end. We also show the replication potential of this system by using small RNA fragments and one template where the product of the first templated ligation step acts as the template for the next, creating a ligation chain reaction.

# 9:25 9:45

### 59

# Consideration on the role of coenzymes in the evolution of Life

### Kirschning A<sup>1</sup>

<sup>1</sup>Leibniz University Hannover

The evolution of coenzymes, or the impact of coenzymes on the origin of Life, is fundamental for understanding our own existence and yet, this topic is rarely discussed in contemporary science. Coenzymes are small molecules that occupy an elementary role with respect to chemical reactivity and selectivity when associated with a macromolecular template. They are essential for functional biocatalysis in all living organisms and act as currency to regulate many basic metabolic processes. Many coenzymes have a simple chemical structure and are often nucleotide-derived, which suggests that they may have co-existed with the emergence of RNA and may have played a pivotal role in early metabolism. Based on current theories on the prebiotic evolution which attempt to explain the emergence of privileged organic building blocks, on protometabolic networks such as the reversed TCA cycle and on established biosynthesis of coenzymes, plausible hypotheses on the early role of coenzymes and cofactors in the evolution of Life will be discussed.

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1. A. Kirschning, Coenzymes and their role in the evolution of Life, Angew. Chem. Int. Ed. 2021, 60, 6242 – 6269.

2. A. Kirschning, The coenzyme/protein pair: A neglected "chicken and egg" problem with significance for the origin of life, Nat. Prod. Rep. 2021, 38, 993 - 1010.

3. A. Kirschning, On the evolutionary history of the twenty encoded amino acids, Chem. Eur. J. 2022 accepted.

# Posters Session 3

### 6

# Prebiotic vesicles on a cold early Earth could have encapsulated solutes, and grown by micelle addition after brief cooling below the membrane melting temperature

**Cohen Z<sup>1</sup>**, Todd Z<sup>1</sup>, Catling D<sup>1</sup>, Black R<sup>1</sup>, Keller S<sup>1</sup> <sup>1</sup>University of Washington

Replication of RNA genomes within membrane vesicles may have been a critical step in the development of protocells on the early Earth. Cold temperatures near 0°C improve the stability of RNA and allow efficient copying, leading some researchers to suggest that the first protocells arose in cold-temperature environments. However, at these temperatures, fatty acids (which would have been available on the early Earth) form gel phase membranes that are rigid and restrict mobility within the bilayer. Two primary roles of protocell membranes are to encapsulate solutes and to grow by incorporating additional fatty acids from the environment. Here we test whether fatty acid membranes in the gel phase accomplish these roles. We find that gel-phase membranes of 10-carbon amphiphiles near 0°C encapsulate aqueous dye molecules as efficiently as fluid-phase membranes do, but not after the aqueous solution is frozen (at -20°C). In contrast, gel-phase membranes do not grow by micelle addition. Growth resumes when membranes are warmed above the gel-liquid transition temperature. We find that longer, 12 carbon amphiphiles do not retain encapsulated contents near 0°C. Together, our results suggest that protocells could have developed within environments that experience temporary cooling below the membrane melting temperature, and that membranes composed of relatively short chain fatty acids would have had an advantage as temperatures approached 0°C.

# Heat flows as a prebiotic driving force of a natural origin-of-life-laboratory

### Mast C<sup>1</sup>

#### <sup>1</sup>Lmu

Prebiotic chemistry often requires certain ratios of ionic species to function. In natural environments, such as those created by the leaching of geomaterials, these requirements are difficult to meet. Examples are basaltic leaches, which contain more sodium than magnesium ions, inhibiting ribozyme function. Another problem is to bring sufficiently high phosphate concentrations, e.g. from apatite, into solution and to prevent its co-precipitation with calcium at non-acidic pH. A possible solution to these issues are lateral heat fluxes through thin, water-filled fractures such as those found in thermally stressed basaltic glass. This non-equilibrium process inverts both the concentration-ratio of sodium to magnesium and that of calcium to phosphate by the heat-driven convection of the solvent and the thermophoretic drift of dissolved ion which is strongly charge and size selective. We show that the excess magnesium thus produced allows ligase ribozymes to function. In the case of dissolved apatite, the thermophoretic separation of calcium and phosphate allows the phosphate to remain in solution even after pH neutralisation and to be concentrated over several orders of magnitude by further heat flow processes. This widely available and geologically plausible scenario could thus help to create the ionic conditions necessary for prebiotic chemistry.

#### Coexistence and evolution of replicators in Metabolically Coupled Replicator Systems (MCRS)

#### Konnyu B<sup>1</sup>

<sup>1</sup>Centre for Ecological Research

Metabolically Coupled Replicator Systems (MCRS) are a model-family in which a simple, physio-chemical and ecologically feasible scenario can be used to study the first steps of the emergence of early replicators communities and proto-cells. The basic idea of the MCRS is that replicators compete for monomers during their replication and, at the same time, replicators cooperate within a reaction network to catalyze their own monomers. During early evolution mineral surfaces created ideal circumstances for synthesis of longer replicators (e.g. RNAs) with three dimensional structure that correspondingly also might have had enzymatic activities. All replicators were in strong competition for monomers during the replication. Those replicators that supported somehow their own monomer supply (e.g. catalyzed a reactions in the monomer synthetic-pathway) might have created a replicator community with indirect interactions among them by the monomer supply and this community excluded all other replicators and communities that they were not so effective like that. All abstract and more realistic variants of the MCRS demonstrate that metabolically active replicators can maintain permanently and replicators are capable of evolving to develop more efficient communities. Furthermore the parasites of the system are not harmful but they are rather pre-adaptive member of the community as we show in this presentation.

# Meteorites and the RNA World: Synthesis of Nucleobases and Ribose in Carbonaceous Planetesimals

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The origin of life might be sparked by the polymerization of the first RNA molecules in Darwinian ponds during wet-dry cycles. The nucleobases and the sugar ribose are key life-building blocks and were found in carbonaceous chondrites. Their exogenous delivery onto the Hadean Earth could be a crucial step toward the emergence of the RNA world. Here, we present the formation of these prebiotic organics through the Strecker synthesis and a simplified version of the formose reaction inside carbonaceous chondrite parent bodies. By using a coupled physico-chemical model, we calculate the abundance of these molecules within planetesimals of different sizes and heating histories. We perform laboratory experiments using catalysts present in carbonaceous chondrites to infer the yield of ribose among all pentoses forming during the formose reaction. These laboratory yields are used to tune our theoretical model that can only predict the total abundance of pentoses. We found that the calculated nucleobase and ribose abundances were similar to the ones measured in carbonaceous chondrites. In conclusion, the Strecker synthesis and aqueous formose reaction might produce most of these organics in carbonaceous chondrites. The life-building blocks of the RNA world could be synthesized inside parent bodies and later delivered onto the early Earth.

# An Amyloid-Centric View of the Prebiotic Origin of Molecular Complexity

**Rout S<sup>1</sup>**, Bomba R<sup>1</sup>, Kwiatkowski W<sup>1</sup>, Greenwald J<sup>1</sup>, Riek R<sup>1</sup> <sup>1</sup>Laboratory of Physical Chemistry, ETH Zurich

The origin of life presents a series of conundrums, one of which is the question of how "prebiotic" molecules became organized into more complex systems of interacting molecules. We have been pursuing the hypothesis that simple peptide aggregates known as amyloids have inherent properties that can explain many questions regarding the origin of molecular complexity. Along the way, we have found that amyloids can chemically self-replicate and self-assemble inside of a protocell as well as specifically bind to codon-sized RNA molecules in a mutually stabilizing interaction.

# Quantum Mechanical Exploration of Prebiotic Chemical Reaction Networks

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Exhaustive computational explorations of prebiotic chemical reaction networks are now within reach due to recent developments of automated quantum mechanical exploration software [1-4]. With our SCINE Chemoton [5,6] computer program, we are able to to probe hypotheses of abiogenesis without the need to perform potentially complex and resource-intensive laboratory experiments. At the same time, we obtain detailed mechanistic and kinetic information about viable production (and decomposition) paths of biochemically relevant molecules. We can study whether and to what extent more complex molecules are formed from simpler building blocks, along which pathways they are formed, and whether they are stable in a given chemical environment [7-9].

Here, we present the SCINE Chemoton software for the automated exploration of chemical reaction networks and show first results for the exploration of two prototypic prebiotic systems, namely the formose network [6] and a Urey-Miller-type network starting from methane, ammonia, water, dihydrogen, and dinitrogen.

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[8] Jonny Proppe and Markus Reiher, "Mechanism Deduction from Noisy Chemical Reaction Networks", J. Chem. Theory Comput., 2018, 15, 357.

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Stereoselective Peptide Catalysis in Complex Environments – From River Water to Cell Lysates [1]

**Rackl J<sup>1</sup>**, Schnitzer T<sup>1</sup>, Wennemers H<sup>1</sup> <sup>1</sup>*ETH Zurich* 

Peptides have been recognized as powerful catalysts for various reactions throughout the last two decades.[2],[3] Of these peptide catalysts, several are characterized by a high degree of stereoselectivity and reactivity. Similar to nature's catalysts, enzymes, they are also composed of amino acids but have a much lower molecular weight and could hence be considered 'mini- enzymes'. Whilst enzymes function splendidly at low concentrations in complex aqueous biological environments, peptide catalysts normally require pure organic solvents and high concentrations.[4a-h]

We were therefore intrigued by the question of whether a peptide catalyst could exhibit chemoselectivity in similar environments reminiscent of enzymes. Consequently, we probed the behavior of tripeptide catalysts in both hydrophobic and aqueous reaction media and further challenged the catalysts with complex reaction media, consisting of aqueous solutions, containing biomolecules, bearing functional groups that can coordinate or react with the catalyst, substrate, or intermediates. Finally, we subjected the peptide catalysts to the ultimate test by investigating their reactivity, chemoselectivity and stereoselectivity in cell lysate in micromolar concentrations, entering a range also typical for enzymes. Despite its relatively short length and small size, H-DPro-  $\alpha$ MePro-Glu-NHC<sub>12</sub>H<sub>25</sub> proved to be a conformationally well-defined tripeptide, able to catalyze C-C bond formations with high reactivity and stereoselectivity, independent of the solvent and its compound composition. In fact, this peptide yielded our desired product with excellent stereoselectivity ( $\geq$  93% ee, d.r. 85:15 - 94:6) and yield (80 - 97%), even in cell lysate, a highly complex mixture with numerous compounds that could either react or coordinate to the catalyst, the substrates, or the reaction intermediates. These findings provoke the question of the potential role of peptide catalysis in nature and during the evolution of enzymes.

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# Si isotopes of microbially induced clay minerals: Exploring a new biosignature for the search for life on Mars

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The 'Rosalind Franklin' rover of the ESA-led ExoMars mission will land on Mars with the goal of possibly finding evidence for the existence of extraterrestrial life. The rover will land at Oxia Planum, an area of Mars that has been selected as a promising site where to look for biosignatures. Indeed, orbital spectral analyses have shown the area to be rich in Fe- and Mg-rich phyllosilicates, matching spectra of smectite, vermiculite and saponite. The presence of these clays, which likely formed at low temperature in the presence of liquid water, points to the existence of a paleoenvironment that may have hosted microbial life. Moreover, experimental studies have shown that authigenic clay precipitation in an aqueous environment can be mediated by the presence of organic compounds and functional groups usually produced by living organisms. We have conducted a series of clay synthesis experiments aimed at expanding upon the organic compound-induced Mg-rich smectite synthesis carried out by Bontognali et al. (2014), with the aim of analyzing the Si stable isotope composition of the resulting silicate precipitates. Our hypothesis is that the presence of organic compounds during authigenic clay precipitation creates a kinetic fractionation of Si isotopes. Varying Si isotope signatures in the presence or absence of organic compounds could serve as a benchmark for the development of a new biosignature. Ultimately, this could be applied to Martian phyllosilicates – obtained from a future Mars sample return mission – in order to investigate the possibility of organic compounds being present upon their formation. This would have considerable implications for the search for life on Mars.

# The Marslabor of the University of Basel: Acquiring close-up images of geological samples in view of the ExoMars rover mission

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The exploration of Mars may finally lead to find an answer to the fundamental question "Are we alone in the universe?". Detecting any form of extant or extinct life on the Red Plant would provide key insight about the origin and distribution of life in the universe. Looking for signs of life on Mars is the main goal of the ESA-led ExoMars rover mission. Here, we describe the preliminary results of some ongoing missionpreparation activities, which are aimed at increasing the scientific return of one of the instruments that will be part of the rover payload, a close up imager called CLUPI. The instrument will be used to take high magnification images of rock textures and sedimentary structures. Such photographs will be of key importance to select interesting samples that will subsequently be analyzed by other instruments placed inside the rover, characterizing the mineralogy and, if present, detecting organic molecules. In view of the prime mission on Mars, we established and indoor facility – the Marslabor of the University of Basel – that has been built ad hoc for simulating a Martian landscape and a Martian illumination. By varying the working distance and light conditions it has been possible to perform an assessment of the minimal-workingdistance required for interpreting rock textures and sedimentary structures that are potentially present at the landing site of the ExoMars rover (i.e., Oxia Planum). The collection of selected rocks includes early Archean microbially induced sedimentary structures (MISS) and other evaporitic minerals and clay-rich sediment that have a high potential of preserving biosignatures. The produced dataset will be of help to the science team for optimizing CLUPI and rover operations during the mission on Mars.

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# Emergence of structure in oligomers originating from templated polymerization of biased pools

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Whether and how structure emerges in random or semi-random nucleic acid pools is a central question in the origins of life. Previously, templated ligation of random AT binary DNA strands has been studied and was found to lead to a reduction of sequence space through selection mechanisms such as avoiding hairpin forming sequences and favoring of A rich and T rich sequences.

We studied polymerization of 12 nucleotides long DNA oligomers of random binary composition (AT or GC) in a model system with Bst enzyme and obtained product strands longer than 100 bp. Analysis of these products through next-generation sequencing revealed the emergence of sequence structure such as self-complementarity and zebraness for AT and favoring of bulky motifs for GC.

How initial composition affects sequence space diversity was investigated by using biased binary pools where the initial fraction of one nucleotide is skewed. Kinetics permitted to ascertain the dependence of length and structure on elongation mechanisms.

In the near future, an analysis of k-motif entropy and motif correlations should allow us to better understand the propagation of information within a sequence. It should also reveal at which scale traces of the initial sequence persist throughout the elongated sequence. This would enable us not only to observe the reduction of sequence space through polymerization, but also to identify possible mechanisms by which it is introduced.

## Heat flows shift chemical equilibria by selective accumulation of ions

**Matreux** T<sup>1</sup>, Aikkila P<sup>1</sup>, Schmid A<sup>1</sup>, Le Vay K<sup>3</sup>, Raith J<sup>2</sup>, Kühnlein A<sup>1</sup>, Weller D<sup>4</sup>, Rappold M<sup>1</sup>, Dingwell D<sup>4</sup>, Altaner B<sup>2</sup>, Guyot F<sup>5</sup>, Gerland U<sup>2</sup>, Scheu B<sup>4</sup>, Mutschler H<sup>3</sup>, Braun D<sup>1</sup>, Mast C<sup>1</sup> <sup>1</sup>Systems Biophysics, LMU Munich, <sup>2</sup>Physics of Complex Biosystems, TU Munich, <sup>3</sup>Biomimetic systems, TU Dortmund, <sup>4</sup>Earth and Environmental Sciences, LMU Munich, <sup>5</sup>Muséum National d'Histoire Naturelle

The first steps in the emergence of life on Earth occurred on rocks and their constituent phases with a feedstock of simple molecules. Our aim is to combine this background with thermal non-equilibrium and bring together geomaterials, chemistry and microfluidics in a realistic environment.

Our experiments take place in reaction chambers, sandwiched between highly heat conducting sapphire plates that ensure complete thermal control including possible thermal gradients. Microfluidic structures are made from FEP, which lets us focus on the interactions between the molecules.

In this scenario, we see that ions leached from prebiotically plausible mineral samples are selectively accumulated by ubiquitous heat flows. Magnesium ions get enriched over Sodium ions and permit ribozyme activity [1]. Thermal non-equilibrium boundary conditions drive concentration gradients, generating and controlling pH gradients in a generally available setting.

Local gradients driven by heat fluxes offer unique opportunities to enable molecular selection on all levels: for simple salts, we see that Phosphate and Calcium are fractionated, making orthophosphate from Apatite available for chemical reactions even at neutral pH. For small organic molecules (such as nucleotides, RNA precursors and amino acids), we observe thermophoretic selectivity for a large pool of molecules (50+). Even for 1-atom differences and same masses, we find that heat flows can drive separation. For larger oligomers, they possibly drive evolution towards functional phenotypes at the origins of life.

[1] Matreux, T., Le Vay, K., Schmid, A. et al. Heat flows in rock cracks naturally optimize salt compositions for ribozymes. Nat. Chem. (2021). https://doi.org/10.1038/s41557-021-00772-5

# Short peptide amyloids are likely a sequence pool for emergent proteins.

**Kwiatkowski W<sup>1</sup>**, Greenwald J<sup>1</sup>, Riek R<sup>1</sup> <sup>1</sup>*ETH* 

Our recent work has shown that amyloids can spontaneously form inside vesicles creating membrane enclosed complex structures of certain degree of variability. This is possible because fatty acids act as filters allowing passage of certain aminoacids and their activated form and as a barrier where aminoacids created from activated species or sequences of aminoacids synthesises inside are becoming non permeable and trapped in the vesicles. It is hypothesized that such preselected sequences become a sequence pool for the emergent proteins. During millions of years of evolution sequences in the current proteome diverged significantly from the original seeds but if the hypothesis is right we should see the trace of them in the current proteome. Here we show that if we find all 6,7,8,9-mers in the proteome and calculate their amyloidogenicity there are more amyloidogenic sequences in the current proteome than in the randomly created proteome of the same size. Moreover, there are more amyloidogenic sequences in archaea proteome than in primate proteome suggesting that the evolution of the proteome is towards a smaller number of amyloidogenic sequences.

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# The surface chemistry of oxides: catalytic activation of the small molecules point of view

**Yakimov A<sup>1</sup>**, Copéret C<sup>1</sup> <sup>1</sup>ETH Zurich

Activation and transformation of the small molecules, e.g. CO2, CH4, CH3X and N2, is challenging to their high stability under ambient earth conditions. In this context, our group and others have shown that the surfaces of oxide materials, e.g. alumina, aluminosilicates, that are ubiquitous on earth, can readily coordinate, activate and catalytically convert such small molecules under relatively mild conditions, in contrast to what may be observed in solution. This can originate from several possibilities: the presence of reactive centers on surface (sites with low coordination numbers, vacancies, frustrated Lewis acid pairs etc.) as well as thermodynamically driven adsorption, that enables a concentration increase of molecules at the surface, leading to a higher probability of reaction between them and increase kinetics.

While most of our research has been motivated by the fundamental understanding of the structure and reactivity of surfaces, in particular how C-C bonds can be formed on surfaces from C1 molecules, one could easily imagine that these processes could be connected to the emergence of first organic molecules on earth and elsewhere.

In this contribution, we summarize the most prominent works of our group on the small molecules activation on the oxide surfaces. We address the structure of the reactive surface sites and the reaction intermediates observed by the state-of-the-art spectroscopic instrumental techniques. Finally, we demonstrate insights into the mechanisms of chemical transformations at the surface obtained using experimental evidences, further augmented by quantum chemical calculations.

As an example, the activation of the C-H bond in CH4 was shown to occur on alumina and silica-alumina surfaces already in 1965 by means of indirect kinetic measurements using CD4. With the development of spectroscopic techniques and quantum chemical calculations in last decades, we were able to show by combining in situ IR spectroscopy complemented by solid-state nuclear magnetic resonance (ss-NMR) spectroscopy and density functional theory (DFT) calculations that tri-coordinated aluminum sites are highly active for this reaction. We have later shown that such surface sites also convert dimethyl ether (CH3OCH3) into higher hydrocarbons. More recently, we have shown that highly isolated Cu(II) sites on alumina surfaces readily convert CH4 into CH3OH, paralleling what nature does using the respective mono-oxygenases.

# Day 3, Thursday, 1.9.2022

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Laukien F<sup>1</sup> <sup>1</sup>Harvard University

# Poster Session 4

29 Arts and Humanities Scholarship in Origin and Prevalence of Life Research

**Davison A<sup>1</sup>** <sup>1</sup>University Of Cambridge, <sup>2</sup>Center of Theological Inquiry

# Talks

#### **KEYNOTE**

Life as a matter of function

#### Petra Schwille1

<sup>1</sup>Max Planck Institute

Compared to physics and chemistry, biology has always been lacking something like a simplified model system such as the hydrogen atom that would allow to formulate and scrutinize first principles and laws required for a fundamental understanding of the phenomenon of life. The reason is that biology's study object is a moving target, as life ever since its origin on earth several billions of years ago has been complexifying through evolution, and although there is the conceptual agreement that the cell should be considered the basic unit of life, nothing is "basic" about this unit, the smallest representations of which still are incomprehensively complicated chemical reaction systems with more than thousands of genes alone. Our hypothesis is that if one ever wants to have in hands and under the microscope a truly minimal living system, one will have to build it from scratch. In contrast to origin-of-life research, however, we do not focus too strongly on the actual molecules nor aim to reproduce the plausible series of events that presumably led to the life we find on earth today. Instead, we understand life as a organizational form of matter that is primarily distinguished by a set of key functions, which can however be abstracted from their specific representatives in various organisms. In the past years, it has been our ambition to identify such a set of key functions for one of life's most central features, self-division. Our experimental work focuses on the reconstitution of a dramatically reduced number of elements of the bacterial cell division system, which however appear to emerge basic features of division in protocell compartments. From our work so far that I will present in my talk, we feel encouraged to believe that the complex cellular division machineries may indeed be deduced to a very limited set of general functional elements, and that some of these rudimentary functions may even still be partly conserved in "modern", highly specialized, proteins.

# 10:55 - 11:15

# 25

# Biogenesis: evaluating fundamental timescales

#### Sasselov D<sup>1</sup> <sup>1</sup>Harvard University

How long does it take for the first viable living cells to emerge on a planet? Recent experiments in prebiotic chemistry and their overlap with insights from the geochemical records of early Earth and Mars allow for evaluation of some fundamental timescales. Many questions remain open, but new experiments are underway.

# 11:15 – 11:35

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Prebiotic Peptide Synthesis and Spontaneous Amyloid Formation Inside a Proto-Cellular Compartment

Kwiatkowski W<sup>1</sup>, Bomba R<sup>1</sup>, Afanasyev P<sup>1</sup>, Böhringer D<sup>1</sup>, Riek R<sup>1</sup>, **Greenwald J<sup>1</sup>** <sup>1</sup>*Eth Zürich* 

Cellular life requires a high degree of molecular complexity and self-organization, some of which must have originated in a prebiotic context. Here, we demonstrate how both of these features can emerge in a plausibly prebiotic system. We found that chemical gradients in simple mixtures of activated amino acids and fatty acids can lead to the formation of amyloid-like peptide fibrils that are localized inside of a protocellular compartment. In this process, the fatty acid or lipid vesicles act both as a filter, allowing the selective passage of activated amino acids, and as a barrier, blocking the diffusion of the amyloidogenic peptides that form spontaneously inside the vesicles. This synergy between two distinct building blocks of life induces a significant increase in molecular complexity and spatial order thereby providing a route for the early molecular evolution that could give rise to a living cell.

# 11:35 – 11:55

### 64

Membraneless Biocondensate Hypothesis prior to Protocells near the Origins of Life, The Evolution of Evolutionary Processes over 3.8 Billion Years towards Feedback-Driven Actively Accelerated Organismal and Real-Time Cancer Evolution

Laukien F<sup>1</sup> <sup>1</sup>Harvard University

The origins of life under driven non-equilibrium conditions require evolvable information-storage macromolecules, either membrane-bound vesicles or protocells, or alternatively membraneless biocondensates generated by liquid-liquid phase separations (LLPS), soon followed by energy metabolism.

The evolution of early life and of contemporary viruses has been driven in significant part by random genetic mutations, while modern unicellular and organismal evolution primarily leverages evolved, efficient and active cell biology processes for adaptive changes prior to selection. Random mutations are often buffered by cell homeostasis, or they have a negative role, e.g., by causing death or monogenic diseases, or by triggering real-time cancer evolution. Accordingly, the Modern Synthesis theory no longer adequately describes the efficient, often punctuated and at times directionally adaptive natural genetic engineering (NGE) processes deduced from the DNA record of evolution.

Early life and advanced life organismal evolution has many parallels with real-time cancer evolution in a host, and they can inform each other. The somatic mutation theory (SMT) of cancer describes driver mutations that can trigger oncogenesis, and passenger mutations characteristic of periods of genetic microevolution in cancer. At the precancerous stage, most somatic mutations are repaired or buffered in the cell, aberrant cells are removed, or organismal bioelectric tissue signals or other physiological functional networks maintain control of rogue, mutated cells. However, the SMT is not sufficient to describe the observed punctuated macroevolution of cancer-cell genes, chromosomes, karyotypes and epigenomes, nor of expressed cancer-cell transcriptomes, proteomes and epiproteomes, which include non-DNA-templated posttranslational modifications, protein-protein interactions and metabolites. Moreover, punctuated cancer cell macroevolution often culminates in macro-effects, which include epithelial-mesenchymal transitions (EMT), cancer cell polyploidies and even giant multinucleated cancer cells that drive cancer progression, therapy resistance and metastasis. All of this cancer-cell evolution competes in a molecular and cellular arms race with host immune cells and antibodies, as well as with the host tumor microenvironment.

Empirically observed punctuated, multilevel and multiclonal cancer macroevolution, and the concomitant, rapid co-development of the host immune system and tumor micro- environment, can occur with the efficiency, speed and lethality of cancer that is enabled by evolved, active natural genetic engineering (NGE) mechanisms. NGE affects both vertical cancer-cell genomic inheritance and evolution towards therapy resistance and metastasis, as well as viral or cancer-cell exosome vector-driven horizontal gene transfers that contributes to cancer cell cooperation, or to transforming previously noncancerous somatic cells into destabilized cancer cells during metastasis.

In addition, externally driven, irreversible and transferable (EDIT) adaptations are exemplified by mitotically heritable, non-templated cancer cell epigenetics, and by mitotically heritable cancer-cell surface protein and lipid glycosylation, as important examples of fast time-scale molecular evolution mechanisms in which genes are followers, similar to evo-devo processes in organismal evolution.

# Poster

### 29

# Arts and Humanities Scholarship in Origin and Prevalence of Life Research

#### Davison A<sup>1</sup>

<sup>1</sup>University Of Cambridge, <sup>2</sup>Center of Theological Inquiry

The origin and prevalence of life in the universe are topics of great significance for the arts and humanities, as well as for the natural sciences. One can easily appreciate that scholars in the arts and humanities who have an interest in these themes ought to attend to research and theories put forward by scientists: in thinking about these matters, they should to be up-to-date with the state of scientific knowledge. The exchange can also run in the other direction, however, with the arts and humanities offering resources for the community of natural scientists working on the origin and distribution of life. Centuries of thinking in the humanities about the nature of life are likely to offer fresh perspectives for the necessarily creative work of interpretation involved in thinking about processes of life beyond our own experience. This poster will present some of the fruits of thought about the place of arts and humanities perspectives in this field that has gone into the foundation of the Leverhulme Centre for Life in the Universe at the University of Cambridge. Particular emphasis will be placed on the potential for philosophical exploration of core concepts that animate this work – ideas such as 'origin', 'pathway', or 'matter' – to offer new perspectives. It will also point to the capacity for philosophy to serve as a bridge between scientific questions and some useful, and more philosophical, areas of mathematics, such as game theory and the exploration of complexity. It is hoped that this poster will serve as a bridge between the work convened in and around Zürich and the burgeoning arts and humanities dimensions to work in Cambridge.

# Day 3, Thursday, 1.9.2022

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# 13:30 - 14:10

#### **KEYNOTE**

# Multicellularity: Biological and Planetary Perspectives

Andrew Knoll<sup>1</sup> <sup>1</sup>Harvard University

The cell is the fundamental unit of life on Earth. The first organisms were most likely unicellular, and numerous clades still complete their life cycles as single cells. That said, multicellularity has arisen many times within Bacteria as well as the Eukarya. Most of these clades can be described as simple multicellular organisms, with cell-cell adhesion but limited communication or differentiation. In these organisms constituent cells remain in more or less direct contact with the external environment, at least during metabolically active stages of the life cycle, and death of individual cells may have only limited impact on the organism as a whole. In contrast, complex multicellularity, defined here operationally as organisms with tissues or organs that circumvent the limitations of diffusion, combine cell-cell adhesion, directed communication between cells and a program of cell differentiation. Organ or tissue failure can doom the whole organism. Such organisms have evolved only about half a dozen times, all within the Eukarya: animals, plants, florideophyte red algae, kelps, and two or more groups of fungi.

While the evolution of multicellularity is a question of biology, it is also one of planetary development, a question of history as well as process. Indeed, a glance at history illuminates the importance of planetary development. While Earth has been a biological planet for most of its history, complex multicellular organisms have populated only the last fifteen percent of that span. Simple multicellular eukaryotes occur in rocks as old as 1600 million years, their evolution perhaps facilitated by resource acquisition, improved predation, or defense against predators. Complex multicellular marine organisms appear ca. 600-575 Ma, coincident with an apparent reorganization of the phosphorus cycle and increases in both primary production and pO2. Thus, energetics, modulated by ecology and rooted as much in planetary as in physiological processes, may lie at the heart of macroscopic diversity on Earth-like planets.

## 14:10 - 14:30

### 33

# Thermal adaptation evolution of the biosphere regulates Earth's longterm climate

**Rogger J<sup>1</sup>**, Mills B<sup>2</sup>, Gerya T<sup>1</sup>, Pellissier L<sup>1</sup> <sup>1</sup>ETH Zürich, <sup>2</sup>University of Leeds

Sustained habitable conditions and the evolution of complex life on Earth depend on efficient climate regulation mechanisms that keep carbon fluxes between geologic reservoirs and the atmosphere-ocean system in balance. The terrestrial biosphere plays an important role in regulating the long-term climate by controlling burial rates of photosynthetically fixed CO<sub>2</sub> as well as by mediating CO<sub>2</sub> consumption through silicate mineral weathering during plant nutrient acquisition, balancing out carbon inputs to the atmosphere-ocean system by volcanism or metamorphism. Current biogeochemical models of the Phanerozoic Earth neglect that the strength of the impact of the terrestrial biosphere on global carbon fluxes is subject to evolutionary dynamics and that it depends on how well the biosphere is adapted to prevailing environmental conditions [1]. Here, we develop a theoretical model to reconstruct million-yearly global organic and inorganic carbon fluxes over the last 400 Myrs. We show that the speed of evolutionary adaptation of the terrestrial biosphere to climatic shifts strongly affects the long-term atmosphere-ocean carbon mass balance. When considering a slow rate of thermal adaptation of the biosphere, resulting in reduced organic carbon burial and especially, strongly reduced silicate weathering rates following temperature shifts, a closer balance of reconstructed Phanerozoic carbon inputs and outputs to and from the atmosphere-ocean system is obtained. Such a balance is a prerequisite to maintain habitable conditions on Earth's surface on a multi-million-year timescale. We argue that the climate evolution of the Phanerozoic Earth is strongly defined by biological and evolutionary processes. Understanding these biological dynamics and how they shape the interactions between Earth's biosphere, geosphere and the climate system may help to understand large shifts in Phanerozoic temperatures and the development of the atmospheric composition of the planet.

[1] Mills, B.J. et al. Modelling the long-term carbon cycle, atmospheric CO<sub>2</sub>, and Earth surface temperature from the late Neoproterozoic to present day. Gondwana Research 67, 172-186. DOI: 10.1016/j.gr.2018.12.001

### 41

# Ediacaran Community Development Suggests a Stochastic Influence on the Early Evolution of Animals

**Stephenson N<sup>1</sup>**, Delahooke K<sup>1</sup>, Kenchington C<sup>1</sup>, Manica A<sup>1</sup>, Mitchell E<sup>1</sup> <sup>1</sup>University Of Cambridge

Modern-day community and ecosystem evolution on Earth is driven by predictable differential patterns in biotic and abiotic variables. Communities develop via succession processes which are largely niche driven. However, previous research has now shown that the first animal communities on Earth were dominated by neutral processes, with stochastic reproduction and dispersal overwhelmingly influencing evolution. It is therefore not known whether community development occurred in early animal communities and what this meant for community dynamics and evolution of the first animals. Here, we show that early animal systems did experience a maturation process, but that there are no consistent signals of composition or individual species dominance. We propose that randomness in community development had a profound effect on the evolution of the first animal life on Earth, rather than the directional and systematic dynamics observed in modern ecosystems. Early animals would therefore not have been predictably exposed to the same combinations of different species, but instead encountered random variation leading to irregular patterns of interactions and evolutionary pressures within a community. This random variation suggests that the point at which systematic niche processes became dominant in animal ecosystems on Earth may be impingent on random biotic and abiotic events. The influence of stochastic events on evolution indicates that the transition from neutral- to niche-dominance on Earth was likely temporally unpredictable, and as such evolutionary dynamics on other planets may not replicate an Earth-like system. Therefore, without the specific evolutionary events that happened on Earth, life on other planets may be markedly different dependant on planet-specific dynamics that drive evolution.

# 14:50 - 15:10

### 50

# The costs and benefits of multicellular group formation in algae

Kapsetaki S<sup>1,2</sup>, West S<sup>2</sup>

<sup>1</sup>Arizona State University, <sup>2</sup>University of Oxford

The first step in the evolution of complex multicellular organisms involves single cells forming a cooperative group. Consequently, to understand multicellularity, we need to understand the costs and benefits associated with multicellular group formation. We found that in the facultatively multicellular algae Chlorella sorokiniana: (1) the presence of the flagellate Ochromonas danica or the crustacean Daphnia magna leads to the formation of multicellular groups; (2) the formation of multicellular groups reduces predation by O. danica, but not by the larger predator D. magna; (3) under conditions of relatively low light intensity, where competition for light is greater, multicellular groups grow slower than single cells; (4) in the absence of live predators, the proportion of cells in multicellular groups decreases at a rate that does not vary with light intensity. These results can explain why, in cases such as this algae species, multicellular group formation is facultative, in response to the presence of predators.

# 15:10 - 15:30

### 67

### How BioEncounters at the microscale prime microbial interactions

### Slomka J<sup>1</sup>

#### <sup>1</sup>ETH Zurich

Microbial life critically depends on cell-cell or cell-resource encounters: these microscale processes control the rate of many fundamental ecological and evolutionary functions. A prominent example are the encounters among phytoplankton in the ocean that lead to the formation of marine snow following a phytoplankton bloom, an important process which fuels the "biological pump," the vertical export of carbon to the deep ocean. Another example is horizontal gene transfer between bacteria by conjugation, a key driver of bacterial evolution that is primed by cell-cell encounters followed by a plasmid-mediated gene exchange. Microscale encounters are nearly always modeled as encounters between inanimate spheres, borrowing from physical models of gasses, coagulating colloids and rain formation. However, I will show here that these physics-based approaches fail to account for important traits of microorganisms, for example cell elongation, and I will outline how more realistic models of encounters and aggregation can contribute to our understanding of fundamental ecological and evolutionary processes controlled by microbes. For example, cell shape, in conjunction with buoyancy and turbulence, can increase encounter rates and thus speed up the formation of marine snow by elongated phytoplankton nearly ten-fold: this result provides a mechanistic explanation for the rapid clearance of blooms of elongated phytoplankton species. I will then describe our recent experimental efforts to measure the probability that a bacteriabacteria encounter results in a plasmid transfer – a key parameter that determines the rates of data exchange and thus genetic innovation between bacteria.

# Poster Session 5

## 32

# Exploring the influence of plants on Phanerozoic climate using a deep time dynamic vegetation model

**Gurung K<sup>1</sup>**, Mills B<sup>1</sup> <sup>1</sup>University Of Leeds

Land plants are key contributors to global primary production and influence atmospheric  $CO_2$  levels. Over the Phanerozoic, terrestrial vegetation and its interaction with atmospheric carbon likely exerted control, to some degree, on climate. However, representation of the terrestrial biosphere over geological timescales and paleogeography in biogeochemical models is limited and poorly understood.

Here, we couple a new deep-time vegetation model (FLORA) to a spatially-resolved long-term climatechemical model (SCION [1]). FLORA improves upon the spatial representation of plant productivity over the Phanerozoic. The dynamic feedback created between local climatic conditions and vegetation biomass allows us to explore the impact of vegetation on organic carbon burial and spatial weathering rate amplification, and thus atmospheric CO<sub>2</sub> concentration over the Phanerozoic. We show that continental aridity during the Triassic and Jurassic restricted CO<sub>2</sub> drawdown and created a hotter climate. Conversely, continental dispersal in the Cretaceous allowed the terrestrial biosphere to sequester more carbon, countering high rates of tectonic degassing and mediating climate. By improving the representation of the terrestrial biosphere and creating local climatic interactions, the new SCION predictions better match available proxy data and highlight the importance of a comprehensive vegetation model within long-term climate-chemical models. Further improvements to the model involve the addition of plant functional types, ecological interactions and terrestrial nutrient cycling. Future work aims to use these models to explore the impact of land colonisation and plant evolution on Phanerozoic climate change.

[1] Mills, B. J. W., Donnadieu, Y. & Goddéris, Y., (2021), Gondwana Research 100, 73-86. doi:10.1016/j.gr.2021.02.011

# High-affinity interactions between amino acids and phyllosilicates: Observations from the biosphere-geosphere interface

#### Blattmann T<sup>1,2</sup>, Takano Y<sup>2</sup>

<sup>1</sup>Geological Institute, ETH Zurich, <sup>2</sup>Biogeochemistry Research Center, JAMSTEC

Earthen and extraterrestrial matrices comprise complex mixtures of minerals and organic matter. Among these organic constituents, amino acids represent a commonality in both environments and are widely considered prerequisite to the origin of life (Degens, 1964). Amino acids are composed of amino and carboxyl functional groups associated with a carbon skeleton and exhibit a wide molecular range from hydrophilic to hydrophobic profiles. The affinity between silicates and amino acids is a controlling factor in producing nitrogenous molecule diversity as well as carbon skeletal elongation reactions (Vinogradoff et al., 2020). Cutting edge investigations on geologically recent matrices showcase direct evidence on the role of phyllosilicates for modulating the preservation of amino acids in the sedimentary record. Observed for the first time in nature using techniques developed by teams at ETH Zurich and JAMSTEC using high-resolution chromatographic isolation and subsequent measurement of amino acid-specific radiocarbon, these preservation patterns largely reflect molecular-level interactions consistent with experimental and theoretical knowledge (Blattmann & Ishikawa, 2020). With an organic geochemical approach to the geological principle of uniformitarianism utilizing the present as a key to the past, we posit that these synergetic interactions between organic molecules and silicate minerals operated similarly on primordial Earth with implications for the spatial disposition and chemical stabilization/modification of life's prebiotic building blocks.

#### References:

Blattmann, T.M. & Ishikawa, N.F. (2020) Theoretical amino acid-specific radiocarbon content in the environment: Hypotheses to be tested and opportunities to be taken. Frontiers in Marine Science, 7, 302. Degens, E.T. (1964) Genetic relationships between the organic matter in meteorites and sediments. Nature 202, 1092-1095.

Vinogradoff, V. et al. (2020) Impact of phyllosilicates on amino acid formation under asteroidal conditions. ACS Earth and Space Chemistry 4, 1398-1407.

### 35

### Stochastic versus deterministic drivers of early animal evolution.

#### Mitchell E<sup>1</sup>

#### <sup>1</sup>University Of Cambridge

The evolution of animals was one of the most important evolutionary transitions in the history of life on Earth, with widespread animals appearing around 600 million years ago (Ma) during the Ediacaran time period. However, the drivers behind the origins and early evolution of these animals are unresolved. Fortunately, the eco-evolutionary dynamics of these Ediacaran animals can be investigated because the fossil preservation during this time is exceptional with thousands of these sessile organisms preserved insitu, as censuses of their communities. This exceptional preservation enables the use of quantitative ecological approaches to test the relative importance of stochastic versus deterministic (environmental) processes for Ediacaran community dynamics. In the oldest Ediacaran animal communities, stochastic processes dominate with deterministic processes exerting limited influence, in contrast with the deterministic and niche-dominated dynamics of modern marine ecosystems. The dominance of stochastic processes suggests that early metazoan diversification may not have been driven by systematic adaptations to the local environment, but instead may have resulted from stochastic demographic differences. This stochastic dynamic changes for younger Ediacaran communities, which were heavily influenced by local environmental patchiness, and also saw a significant increase in competition within and between different species. These environmental interactions are deterministic or predictable. Further analyses of all known Ediacaran communities show that throughout the Ediacaran there is increasing environmental specialisation and ecological complexity, paving the way for more familiar animals to rise in the Cambrian. This change in eco-evolutionary dynamics throughout the first animals of the Ediacaran, from stochastic to deterministic, raises the intriguing possibility that other key evolutionary events and dynamics may be a mixture of random chance and predictable responses to the biosphere, and that the origins of animals themselves may not have been inevitable.

# Experimental evolution under extraterrestrial conditions

**McGinnis D<sup>1,2</sup>**, Ibelings B<sup>1,2</sup>, Thomas M<sup>2</sup>, **Bolmont E<sup>1,2</sup>** <sup>1</sup>Center Life in the Universe, <sup>2</sup>University of Geneva

Life is defined by the capacity of Darwinian evolution. Experimental evolution has proven to be one of the most powerful tools to study the mechanisms of evolution on Earth (e.g. Lenski et al. 2017). Evolution that drove the diversification of life from a simple and homogenous beginning. We aim to perform experimental evolution and observe which geno- and phenotypic traits will be favored under conditions found on different planets. For this we assume that there is a core to life that is similar on Earth and elsewhere, so that presently the best model system to study Life in the Universe are life-forms found on Earth. There are many organisms (facultatively) adapted to life in the absence of oxygen (e.g. methanogens, yeast, e.g. Beatty et al. 2005 for an example). Some of these function with very simple substrates, for example methane production occurring from hydrogenotrophic processes, where the substrates could be from expelled biogases of other organisms or by carbonate rock erosion (4H2 + CO2 -> CH4 + 2H2O). These processes also alter the balance of the stable C isotopes in the system ( $\delta$ 13C).

From this perspective, we propose conducting experiments on organism evolution in alternative environments (various substrates and initial atmospheres, such as H2 + N2 mixture or CO2). Besides quantifying the organism's evolutionary trajectory, we propose to monitor - using existing equipment in Department Forel from the university of Geneva - the various gases consumed or produced by these organisms, i.e. to investigate what types of atmospheric gas compositions could suggest the presence of life on extra-terrestrial worlds. Studies have shown growth of unicellular prokaryotes and eukaryotes under conditions found on other planets, like the H2 dominated atmosphere of rocky exoplanets (Seager et al. 2020), so the potential for experimental evolution is present.

We will present this project, which will start in Septembre-Octobre of this year and which will bring elements of answers on two major questions:

- What are the key traits that evolve when life adapts to non-earth like conditions and what is the nature of the underlying mutations?

- What are the biosignatures found as a consequence of the evolution of new traits? Are they unique signatures of life?

51

## Motile cilia and eukaryogenesis by comparative structural studies

Ishikawa T<sup>1,2</sup>, Noga A<sup>1</sup> <sup>1</sup>PSI, <sup>2</sup>ETH Zurich

Cilia are appendage-like organelles of eukaryotes with ~300nm diameter and 5~20  $\mu$ m length. There are two types of cilia – motile and immotile. Motile cilia have unique structure composed of nine microtubule doublets surrounding two single microtubules, called "9+2", and powered by dynein, ATP-driven motor proteins. This 9+2 structure of motile cilia is shared from unicellular algae to human, suggesting that the origin of this organelle is widely common, and maybe can be tracked back to the last eukaryotic common ancestor (LECA). Probably motile cilia were acquired by unicellular cells at the early stage of eukaryogenesis, since they were necessary for them to swim toward light and nutrition, and evolved to be in multicellular organisms with various functions. In human, motile cilia function in tracheae, oviducts, brain, sperm and embryos. Defect of motile cilia causes various diseases (primary ciliary dyskinesia).

Interestingly the base part of cilia, called the basal body, which determines nine-fold symmetry and becomes the seed of ciliogenesis, is the same organelles as centriole, the center of microtubule cytoskeleton for cell division. It is still an open question, either the basal body was recycled as the center of cell division, or the centriole was used to be a core of ciliogenesis. Variety of questions regarding origin of motile cilia are unanswered as well – Were cilia originated from other already existing microtubule-based organelles, or brought by other organisms with endosymbiotic or syntrophic mechanisms? Did motile cilia appear first and evolved to immotile cilia, or vice versa? Etc.

Our group has been working on questions regarding motile cilia and the basal body, using comparative structural studies by cryo-electron microscopy, combined with genetic/phylogenetic approaches. Our structural analyses gave mechanistic insight of motile cilia, but also suggestion how motile cilia have been evolving in the history of eukaryotes. In this presentation, we will show our comparative studies on large motor and regulatory complexes from cilia and discuss from evolutional viewpoints.

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# Day 3 & 4: Thursday, 1.9. 2022 & Friday, 2.9.2022

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<sup>1</sup>Space Research and Planetary Sciences, Physics Institute, University Of Bern, <sup>2</sup>NCCR PlanetS, University of Bern

# **24** Microbial Mat Hosted Gypsum from a Sabkha in Qatar: Raman microscopy and microbial community analysis

**Dittrich M<sup>1</sup>**, Diloreto Z<sup>1</sup>, Shaharyar Ahmad M<sup>1</sup>, Bontognali T<sup>2</sup>, Al Saad Al-Kuwari H<sup>3</sup>, Sadooni F<sup>3</sup> <sup>1</sup>University of Toronto, <sup>2</sup>Space Exploration Institute, <sup>3</sup>Qatar University

#### 30 Implications for Early Earths and Biospheres from Studies of Subglacial Lakes in the Land of Fire and Ice

**Gaidos E<sup>1</sup>** <sup>1</sup>University Of Hawaii At Manoa

#### 61 Metabolic signatures and biomass limits of an aerial biosphere in the clouds of Venus

Jordan S<sup>1</sup>, Shorttle O<sup>1,2</sup>, Rimmer P<sup>2,3,4</sup>

<sup>1</sup>Institute Of Astronomy, University of Cambridge, <sup>2</sup>Department of Earth Sciences, University of Cambridge, <sup>3</sup>Cavendish Laboratory, University of Cambridge, <sup>4</sup>MRC Laboratory of Molecular Biology

# Posters Session 6

**9** Introducing the Cosmic Origins Of Life (COOL) model: a multi-scale, multi-physics framework for the emergence and survival of life in a hostile Universe

**Kruijssen D<sup>1</sup>**, Longmore S<sup>2</sup> <sup>1</sup>Heidelberg University, <sup>2</sup>Liverpool John Moores University

#### 69 Exploring the role of extremophiles for the formation of Mg-rich carbonate minerals

**Al Disi Z<sup>1</sup>**, Zouari N<sup>1</sup>, Dittrich M<sup>1,2</sup>, McKenzie J<sup>3</sup>, Al-Kuwari H<sup>1</sup>, Bontognali T<sup>1,4,5</sup> <sup>1</sup>Qatar University, <sup>2</sup>University of Toronto Scarborough, <sup>3</sup>ETH, <sup>4</sup>Space Exploration Institute (SPACE-X), , <sup>5</sup>University of Basel

#### 901 Microbial sulfur cycling in lacustrine sediments from a mid-Proterozoic Ocean analogue

Paula Rodriguez<sup>1</sup>, Jasmine Berg<sup>2</sup>, Longhui Deng<sup>2</sup>, Hendrik Vogel<sup>3</sup>, Mark A. Lever<sup>2</sup>, Cara Magnabosco<sup>1</sup>

<sup>1</sup>Department of Earth Sciences, ETH-Zurich, Zurich, Switzerland;<sup>2</sup>Department of Environmental Systems Science, ETH-Zurich, Zurich, Switzerland;<sup>3</sup>Institute of Geological Sciences, University of Bern, Bern, Switzerland & Oeschger Centre for Climate Change Research, University of Bern, Bern, Switzerland.

#### 902 Size-dependent cataclastic hydrogen gas production

Andrew Acciardo<sup>1</sup>, Claudio Madonna<sup>1</sup>, Cara Magnabosco<sup>1</sup>

<sup>1</sup>Department of Earth Sciences, ETH-Zurich, Zurich, Switzerland

#### 903 CLUPI/ExoMars, The Search for Past Life on Mars

#### Jean-Luc Josset<sup>1</sup>

<sup>1</sup>Space Exploration Institute, CH-2000 Neuchatel Switzerland

**910** The Bedretto Underground Laboratory for Geosciences and Geoenergies: a new experimental laboratory for studying the extent and prevalence of subsurface life

Cara Magnabosco<sup>1</sup>, Andrew Acciardo, Bernard Brixel, Marian Hertrich, Hansruedi Maurer, Stefan Wiemer, Domenico Giardini

<sup>1</sup>ETH Department of Earth Sciences,

# Talks Session 6

# 16:00 - 16:40

#### **KEYNOTE**

# Life in Extreme Environments: From Rio Tinto to the Ocean of Enceladus

Jonathan Lunine<sup>1</sup> <sup>1</sup>Cornell University

Life exists almost anywhere on Earth that liquid water is present. What can extremophiles teach us about the potential for life in habitable. but still challenging environments such as the ocean of Enceladus and possible hypersaline pockets in Europa? And what about those methane seas on Titan—how can one approach the question of their habitability

# 16:40 - 17:00, 1.9.2022

### 7

# Getting closer to solar flares and coronal mass ejections

#### Harra L<sup>1</sup>

<sup>1</sup>Pmod/wrc & Ethz

Solar flares and coronal mass ejections are currently studied in exceptional detail with new spacecraft launched in the past 4 years which add to the existing fleet. These spacecraft get close to the Sun, and provide an exceptionally detailed view of all scales of activity on the Sun - from the formation of the solar wind to the trigger of large scale flares.

These observations of solar flares and coronal mass ejections allow us to probe what happens to create the environment that surrounds planets, and is a major influence on whether there can be life on other planets. We will summarise the latest developments in the understanding of solar activity, and the future developments that we expect in the coming years with the new missions.

### 62

## Heating planetary bodies with tidal interactions

**Bagheri A**, Khan A, Efroimsky M, Samuel H, Deschamps F, Giardini D <sup>1</sup>*Eth Zurich* 

Tidal evolution is playing a critical role in the development of the architecture of the solar and extra-solar systems. On the one hand, tides add a lot to the n-body interactions in these systems. On the other hand, tidal heating contributes greatly to the thermal processes and internal evolution of planets. Among the numerous examples of the working of tides in the solar system are: (1) the Martian moons Phobos and Deimos, which are migrating towards and away from its host planet, respectively; (2) the Jovian moon Europa with its subsurface liquid ocean; (3) the Saturnian moon Enceladus renowned for its water-rich plumes venting into space. Inarguably, tides and tidal heating are playing a major role in determining planetary habitability. Modeling tidal evolution of orbits and interiors thus becomes a key to our understanding the evolution and current state of planetary systems. We developed a tidal model applicable to describing highly eccentric orbits and higher-order spin-orbit resonances. The tidal model is combined with self-consistently built interior structure models, and is used to explore evolution of both rocky and icy planets and moons. We emphasize on the necessity of taking into account appropriate combined tidal and thermal evolution modeling for constraining the interior properties, and exterior architecture of the planetary systems. Our model has been employed to study, e.g., the orbital evolution of the Martian moons, the Pluto-Charon binary, exoplanet TRAPPIST-1e, and

the dwarf planet Gonggong. We show that the use of this tidal model is essential to obtain precise results. Specifically, we study the importance of the tidal heating in formation and maintaining the subsurface liquid oceans that can be potentially habitable.

# 21

# Enabling the search for life in our solar system with 3D microscopy techniques

**Serabyn E<sup>1</sup>**, Lindensmith C<sup>1</sup>, Wallace K<sup>1</sup>, Liewer K<sup>1</sup>, Kim T<sup>1</sup>, Oborny N<sup>1</sup>, Nadeau J<sup>2</sup> <sup>1</sup>Jet Propulsion Laboratory, <sup>2</sup>Portland State University

The existence of life beyond the Earth can be investigated either spectroscopically, on exoplanets around nearby stars, or in situ, by sending probes to our own solar system's planets, moons and asteroids. In the latter case, in situ microscopic imaging of potential microbes is a promising possibility. Potential environments can range from ices and liquid water on outer solar system moons and asteroids, to shielded regolith and caves on Mars, to aerosols in the clouds of Venus. We will describe 3D microscopy techniques applicable to a variety of environments, including digital holographic microscopy and light-field fluorescence microscopy, that we have been developing to enable the search for cellular life in its native environment on such worlds. Our microscope systems have already been successfully deployed to a number of remote terrestrial sites.

# 9:25 - 9:45

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# Towards In Situ Amino Acid and Lipid Detection on Ocean Worlds using Laser Desorption Ionisation Mass Spectrometry

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The search for and detection of extinct or extant life outside of Earth is a major topic in space sciences. Finding signs of life on extraterrestrial Solar System Bodies could give us important clues of how life could form. Detection of signatures of life, so-called biosignatures, is therefore necessary, but remains a highly challenging task. Instrumentation should be flight-capable, posing several restrictions on weight, dimensions, and power usage. Detection capability should also not be limited to only one compound or group, but should be more broadly applicable to several groups of compounds that are relevant for life. High sensitivity is required as well to detect trace abundances.

Ocean Worlds, such as Europa and Enceladus, are highly interesting to search for signs of life, since all ingredients to form life (as we know it) are present [1]. Plumes, that spray out through cracks in the ice shells, could contain biosignatures, making in direct sampling of the ocean underneath possible. Several groups of compounds are listed as potential targets in the search for life, including amino acids and lipids. Amino acids are the building blocks of proteins, while lipids are involved in cell structure and function. Both are essential compound groups for life as we know it. Detection and identification of both groups is therefore of interest for future space exploration missions in the search for signs of life.

ORIGIN, standing for ORganics Information Gathering INstrument, is a novel prototype laser desorption mass spectrometer (LDMS) and has been designed for in situ space exploration missions [2]. The design is compact and robust and complies with the requirements for space instrumentation. The current setup consists of a nanosecond pulsed laser system and a miniature reflectron-type time-of-flight mass analyser (160 mm x Ø 60 mm) [3]. Sample material is desorbed and ionised and generated cations are separated in the mass analyser based on their mass-to-charge ratio (TOF principle), resulting in a single mass spectrum for each laser pulse.

Measurements of amino acid and lipid standards were performed to assess the capabilities of ORIGIN [2,4]. Standard measurement protocols were established and subsequently used in studies conducted to investigate sensitivity and limit of detection, optimal conditions for laser desorption, and influence of the sample holder substrate. In our contribution, we will discuss the setup, measurement procedures, and present and discuss our latest findings using the ORIGIN prototype. The implications of our results will be discussed with focus on the suitability of the presented technique for future space missions to Ocean Worlds in the search for signs of life.

#### References:

[1] Lunine J.I. (2017) Acta Astronaut., 131, 123-130.

[2] Ligterink N.F.W. et al. (2020) Sci. Rep., 10, 9641.

- [3] Riedo A. et al. (2013) J. Mass Spectrom., 48, 1-15.
- [4] Boeren N.J. et al. (2022) to be submitted.

# 10:15 - 10:35

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# Microbial Mat Hosted Gypsum from a Sabkha in Qatar: Raman microscopy and microbial community analysis

**Dittrich M<sup>1</sup>**, Diloreto Z<sup>1</sup>, Shaharyar Ahmad M<sup>1</sup>, Bontognali T<sup>2</sup>, Al Saad Al-Kuwari H<sup>3</sup>, Sadooni F<sup>3</sup> <sup>1</sup>University of Toronto, <sup>2</sup>Space Exploration Institute, <sup>3</sup>Qatar University

The sabkha environments of Qatar represent a unique opportunity to gain insight into the production and preservation of halophilic biomarkers similar to those that might have occurred on Mars. Sabkhas may be analogous to past evaporitic surfaces of Mars due to their arid location with elevated concentrations of salt, and increased insolation by low-wavelength radiation. Furthermore, sabkhas in Qatar host extensive assemblages of evaporitic minerals, including gypsum in close association with abundant and diverse hypersaline microbial communities.

Evaporitic minerals act as a refuge for extremophilic microorganisms in the extreme environments. Gypsum can offer protection against desiccation, rapid temperature fluctuations, and exposure to UV-radiation, while still allowing the penetration of electromagnetic radiation. On the other hand, gypsum could be a very effective medium for the preservation of biomarkers. Given the elevated levels of UV-radiation on the Martian surface, it is reasonable to postulate that surviving microorganisms would have produced UV-shielding pigments as a major component of their survival strategy. One such pigment of consideration is  $\beta$ -carotene due to its ability to repair damaged DNA and absorb UV-C radiation.

The aim of our work is to better understand the interactions of biomarkers, e. g., pigments that may be preserved within a gypsum matrix and to evaluate a potential of Raman microscopy to detect the biomarkers in gypsum crystals from extreme environment. To better understand the interactions of pigments or other biomarkers encapsulated in a gypsum matrix, sediment cores samples of buried microbial mats and gypsum from the Dohat Faishakh sabkha in Qatar were collected. These samples were evaluated using a combination of microbial DNA analyses to determine organisms present and their aptitude for producing biomarkers, as well as Raman spectroscopy to analyze biomarkers trapped within the gypsum mineral matrix. This study showed that organic material produced by in these environments is encapsulated within gypsum and able to be detected using standard Raman spectroscopic methods with little sample preparation.

## 10:35 - 10:55

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# Implications for Early Earths and Biospheres from Studies of Subglacial Lakes in the Land of Fire and Ice

#### Gaidos E<sup>1</sup>

<sup>1</sup>University Of Hawaii At Manoa

"Extreme" environments provide intellectual inspiration and some ``ground truth" for discussions of conditions and events involved in the emergence and early evolution of a biospheres on Earth and other habitable worlds. Among the factors often considered in such discussions are the availability of chemical energy sources prior to an origin of phototrophy, and emerging feedbacks between biologically-mediated geochemical cycles in a nascent biosphere and climate. Ice-covered lakes are a subset of extreme environments that can offer insight into an ice-covered Earth under a fainter young Sun (and "snowball Earth" episodes) as well as ice-covered oceans in some satellites of giant planets. In Iceland, volcanic heat maintains several subglacial lakes under the Vatnajokull ice cap. These lakes are completely isolated from sunlight and mostly (but not completely) isolated from the atmosphere. Our exploration of these lakes over the past two decades has shown them to be near the freezing point, anoxic, and highly sulfidic, with chemistries that resemble hydrothermal fluids diluted by glacial melt. Moreover, we have detected and described an active microbial biome that is endemic to the lakes and unlike anything described in natural environments elsewhere. Unsurprisingly, we find that that taxa in this biome are related to organisms with established metabolisms able to use the sources of chemical energy in the lake water column, i.e. carbon dioxide, hydrogen, sulfur and (probably) the minor amount of oxygen released into the lake by melting glacial ice. More interesting is the structure of the community, which is dominated by only a few taxa, all bacteria. Unexpectedly, the dominant lithoautotrophic metabolism involving carbon dioxide and hydrogen is not methanogenesis, but acetogenesis. One of the dominant taxa in these lakes is not only capable of acetogenesis as an energy source, but uses this as a source of fixed carbon and is capable of nitrogen fixation as well. Even more surprising is the apparent absence of members of the Archaea, including all known lithotrophic methanogens, i.e. non-detection by multiple methods including metagenomics. The absence of methanogens and the dominance of acetogens (a situation hitherto undescribed outside of termite guts) could be related to specific environmental conditions, i.e. low temperatures and high hydrogen activity. The complete absence of archaea is much more mysterious, and (speculatively) may be related to high energy levels, or insolubility and unavailability of metal cofactors such as Fe in the presence of high sulfide. The enzymes involved in methanogensis and acetogensis appear to be ancient and evolutionarily related. Methane is an important greenhouse gas and a popular biosignature, while acetate would be highly soluble in oceans. On biospheres where conditions favor acetogenesis, such attributes would be absent, with implications for the climate and detection of life elsewhere.

# 10:55 – 11:15

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# Metabolic signatures and biomass limits of an aerial biosphere in the clouds of Venus

#### Jordan S<sup>1</sup>, Shorttle O<sup>1,2</sup>, Rimmer P<sup>2,3,4</sup>

<sup>1</sup>Institute Of Astronomy, University of Cambridge, <sup>2</sup>Department of Earth Sciences, University of Cambridge, <sup>3</sup>Cavendish Laboratory, University of Cambridge, <sup>4</sup>MRC Laboratory of Molecular Biology

Life in the clouds of Venus, if present in sufficiently high abundance, must be affecting the atmospheric chemistry. It has been proposed that abundant Venusian life could obtain energy from its environment using three possible sulfur energy-metabolisms. These metabolisms raise the possibility of Venus's enigmatic cloud-layer SO2-depletion being caused by life. We couple each proposed energy-metabolism to a photochemical-kinetics code and self-consistently predict the composition of Venus's atmosphere under the scenario that life produces the observed SO2-depletion. Using this photo-bio-chemical kinetics code, we show that all three metabolisms can produce SO2-depletions, but do so by violating other observational constraints on Venus's atmospheric chemistry. This therefore enables us to place an upper limit on the maximum allowed biomass in Venus's clouds before the effect of life's energy-metabolism violates observational constraints on the atmospheric chemistry. We calculate the maximum possible biomass density of sulfur-metabolising life in the clouds to be 10^{-5} - 10^{-3} mg m^{-3}, under the assumption that cell maintenance power requirements are high in the extreme environment of Venus's acid cloud layer, compared to cell power requirements of life on Earth. The methods employed are equally applicable to predicting chemical signatures of aerial biospheres on Venus-like exoplanets, planets that are optimally poised for atmospheric characterisation in the near future.

# Posters Session 6

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# Introducing the Cosmic Origins Of Life (COOL) model: a multi-scale, multiphysics framework for the emergence and survival of life in a hostile Universe

**Kruijssen D<sup>1</sup>**, Longmore S<sup>2</sup> <sup>1</sup>Heidelberg University, <sup>2</sup>Liverpool John Moores University

Our existence is arguably the biggest multi-scale astrophysics problem. Not only does it require a comprehensive understanding of the astrophysical processes enabling the emergence of life, but also of the processes that could end it. A comprehensive answer to the problem requires linking galaxy formation and evolution, star formation, stellar feedback, and the formation and evolution of planetary systems. We will present a unified "cosmic planet population synthesis" modelling framework named Cosmic Origins Of Life (COOL), which combines prescriptions for all of these processes to self-consistently predict the emergence and persistence of habitable planets and Earth-like life across cosmic history. COOL connects state-of-theart models for the formation of galaxies, stellar clusters, stars, and their planetary systems, accounting for the multi-scale, multi-physics environmental dependences between these. In addition, it accounts for a wide range of cosmic hazards, including the external photoevaporation and dynamical disruption of protoplanetary discs by nearby stars, dynamical perturbations of planetary systems by stellar encounters, the impact of supernova explosions and GRBs on planets, and asteroids showers, including their dependences on the evolving galactic environment. By self-consistently following stars and planets as they form and evolve within the galactic environment, the model determines the occurrence rate, proximity and magnitude of these hazards for each planetary system. Using this model, we will show which astrophysical threats are the most likely to impact both the solar system and planetary systems in general, as a function of their stellar mass, age, chemical composition, and location. These insights help to answer if we live in the most fertile, benign, and suitable galactic environment and stellar system compared to other galaxies and host stars.
# Exploring the role of extremophiles for the formation of Mg-rich carbonate minerals

**Al Disi Z<sup>1</sup>**, Zouari N<sup>1</sup>, Dittrich M<sup>1,2</sup>, McKenzie J<sup>3</sup>, Al-Kuwari H<sup>1</sup>, Bontognali T<sup>1,4,5</sup> <sup>1</sup>Qatar University, <sup>2</sup>University of Toronto Scarborough, <sup>3</sup>ETH, <sup>4</sup>Space Exploration Institute (SPACE-X), , <sup>5</sup>University of Basel

Mg-rich carbonate minerals, (e.g., dolomite - (Ca,MgCO3) are a common constituent of ancient sedimentary sequences. Studies conducted in the field of geobiology have shown that microbial activity promote the formation of Mg-rich carbonates at low temperature, which implies that some occurrences of such minerals in the geological record may represent a biosignature. This hypothesis is of great interest in the field of research studying the evolution of early life on Earth and for the search of life on other planets. Indeed, dolomite often occurs in Archean rocks in association with putative microbially induced sedimentary structures, and Mg-rich carbonates that likely formed at low temperature have been identified by orbital spectral analysis on Mars (e.g., Marginal Carbonates at Jezero Crater). Here, we present the results of laboratory precipitation experiments that have been conducted with extremophilic microbes isolated from the sabkhas (i.e., salt flats) of Qatar. Specifically, we tested how the presence of cells and extracellular polymeric substances (EPS) with specific functional groups influence the mol% Mg of carbonate minerals that form through evaporation of seawater. We show that high Mg calcite with a mol% of Mg of  $45 \pm 1.2$  precipitates in the presence of EPS or bacterial cells. Instead, a mol% of maximum  $35 \pm 1.8$  was detected in parallel control experiments conducted under identical conditions but in the absence of organic molecules. These results provide insight that allows for better linking Mg-rich carbonates and extremophilic microbes.

Keywords: Bacterial cells, EPS, Functional groups, Protodolomite.

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# Microbial sulfur cycling in lacustrine sediments from a mid-Proterozoic Ocean analogue

Paula Rodriguez<sup>1</sup>, Jasmine Berg<sup>2</sup>, Longhui Deng<sup>2</sup>, Hendrik Vogel<sup>3</sup>, Mark A. Lever<sup>2</sup>, Cara Magnabosco<sup>1</sup>

<sup>1</sup>Department of Earth Sciences, ETH-Zurich, Zurich, Switzerland;<sup>2</sup>Department of Environmental Systems Science, ETH-Zurich, Zurich, Switzerland;<sup>3</sup>Institute of Geological Sciences, University of Bern, Bern, Switzerland & Oeschger Centre for Climate Change Research, University of Bern, Bern, Switzerland.

Lake Cadagno (Ticino, Switzerland) is one of the few sulfidic, meromictic lakes in Europe and is frequently cited as an analogue to the Proterozoic ocean. The water column of the lake contains ~ 2 mM of dissolved sulfate, a concentration 10 times higher than most freshwater basins. However, since the lake's formation following deglaciation, the bottom layer of the water column has undergone redox transitions from oxic, to periodically anoxic, to euxinic. These redox transitions are reflected in the sedimentary record of the lake. Thus, Lake Cadagno sediment constitute an ideal natural setting to study the co-evolution of sediment geochemistry in the subsurface with its associated biosphere. Here, we investigated the potential role of microorganisms in biological sulfur cycling on a 13.5 kyr sediment succession from Lake Cadagno. We sequenced the dissimilatory sulfite reductase beta subunit gene (dsrB) from sediment samples encompassing the last 10 kyr of sediment deposition and found that microorganisms from the class Deltaproteobacteria dominate the organic matter-rich surface sediments above the sulfate-depletion zone. Reconstruction of Deltaproteobacteria genomes from surface sediment metagenomes identified the complete set of genes to perform canonical dissimilatory sulfate reduction (DSR). In contrast, in midcolumn, sulfate-poor sediments, 44% to 98% of the dsrB gene sequences belong to representatives from Dehalococcoidia and Anaerolineae, from the phylum Choloroflexi. Together, these results indicate that active sulfur cycling is occurring in surface and deep lacustrine sediments, although the biochemical mechanisms are still unclear. Further genome-resolved analyses will provide new insights into the role of microbial populations in the biogeochemical sulfur cycling in Lake Cadagno.

#### Size-dependent cataclastic hydrogen gas production

Andrew Acciardo<sup>1</sup>, Claudio Madonna<sup>1</sup>, Cara Magnabosco<sup>1</sup>

<sup>1</sup>Department of Earth Sciences, ETH-Zurich, Zurich, Switzerland

Over 70% of Earth's prokaryotes live in the subsurface. These microorganisms can utilize various electron donors. The simplest of these electron donors is molecular hydrogen, which is thought to have been used by primitive life forms during the earliest stages of life on Earth. In the subsurface, hydrogen can be generated through a variety of water-rock reactions including radiolysis, serpentinization and cataclasis. Cataclastic hydrogen production occurs via a mechanoradical reaction between water and silicate rocks that have been crushed or fractured. To understand the influence of grain size in the mechanoradical production of hydrogen and to calculate an estimate for global cataclastic hydrogen production on Earth, we carried out a series of water-rock reactions with varying sizes of granite rock grains. Grain size distributions of rocks have been shown to decrease as a result of seismic activity, a process which is thought to play a role in earthquake instability. Thus, it is important understand how these size distributions control the level of hydrogen produced and consequently the fates of the microbial communities living within the rocks. Samples of Rotondo granite from a borehole drilled in the Bedretto tunnel in Ticino, Switzerland were hydraulically crushed, milled, and vacuum-sieved into three size-fractions. After initiating the reaction in anoxic glass vials, the headspace was tested to determine hydrogen gas concentration using gas chromatography. After twenty hours of incubation, the 45-63  $\mu$ m, 90-106  $\mu$ m, and 125-150  $\mu$ m size fractions showed net hydrogen production of 142.34±31.34, 103.62±16.75, and 16.93±1.78 nmol g-1 rock, respectively. Control samples with either no rock or no water showed only trace levels of hydrogen. Additional experiments using different lithologies and types of water are also being performed and will help illuminate the influence of mechanoradical hydrogen production for life on Earth as well as potential life on planets and moons in our solar system and beyond.

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### CLUPI/ExoMars, The Search for Past Life on Mars

#### Jean-Luc Josset<sup>1</sup> and the CLUPI Science Team

#### <sup>1</sup>Space Exploration Institute, CH-2000 Neuchatel Switzerland

The main goal of the ExoMars rover mission is the search of life on Mars. The Mission was planned to be launched in September 2022 before to be postponed (in 2028 ?) due to the suspension of collaboration with Russia.

The scientific objectives of the ESA ExoMars rover mission are to search for traces of past or present life and to characterise the near-sub surface. Both objectives require study of the rock/regolith materials in terms of structure, textures, mineralogy, and elemental and organic composition. The key point of the ExoMars rover is the capability to drill the surface of Mars up to 2m under the surface and to collect samples to be in-situ analysed.

The ExoMars rover payload consists of a suite of complementary instruments designed to reach these objectives.

CLUPI, the high-performance colour close up imager, part of the science payload on board the ExoMars Rover plays an important role in attaining the mission objectives: it is the equivalent of the hand lens that no geologist is without when undertaking field work. CLUPI is a powerful, highly integrated miniaturized (<900g) low-power robust imaging system, able to sustain very low temperatures (–120°C). CLUPI has a working distance from 11.5cm to infinite providing outstanding pictures with a color detector of 2652x1768x3. At 11.5cm, the spatial resolution is 8 micrometer/pixel in color. The optical-mechanical interface is a smart assembly that can sustain a wide temperature range.

Given the time and energy expense necessary for drilling and analysing samples in the rover laboratory, preliminary screening of the materials to chose those most likely to be of interest is essential. ExoMars will be choosing the samples exactly as a field geologist does – by observation (backed up by years and years of field experience in rock interpretation in the field). Because the main science objective of ExoMars concerns the search for life, whose traces on Mars are likely to be cryptic, close up observation of the rocks and granular regolith will be critical to the decision as whether to drill and sample the nearby underlying materials. Thus, CLUPI is the essential final step in the choice of drill site. But not only are CLUPI's observations of the rock outcrops important, but they also serve other purposes. CLUPI, could observe the placement of the drill head. It will also be able to observe the fines that come out of the drill hole, including any colour stratification linked to lithological changes with depth. Finally, CLUPI will provide detailed observation of the surface of the core drilled materials collected up to 2m under the surface when they are in the sample drawer at a spatial resolution of about 15 micrometer/pixel in color.

A brief review of the science objectives of the ExoMars mission together with the observation modes of the instrument will be described, showing importance of CLUPI capabilities to provide information, significantly contributing to the understanding of the geological environment and could identify outstanding potential biofabrics of past life on Mars.

#### 903

# The Bedretto Underground Laboratory for Geosciences and Geoenergies: a new experimental laboratory for studying the extent and prevalence of subsurface life

Cara Magnabosco, Andrew Acciardo, Bernard Brixel, Marian Hertrich, Hansruedi Maurer, Stefan Wiemer, Domenico Giardini

#### <sup>1</sup>ETH Department of Earth Sciences,

The Bedretto Underground Laboratory for Geosciences and Geoenergies is located within the ~5km long Bedretto Tunnel in Ticino, Switzerland. The tunnel was originally excavated as part of the construction logistics of the Furka Base Tunnel and traverses the Gotthard Massif, encountering up to ~1.6 km of granitic overburden. In 2018, the ETH Zürich Department of Earth Sciences began developing the Bedretto Underground Laboratory for Geosciences and Geoenergies (BULGG) in collaboration with the Matterhorn Gotthard Bahn and, in 2021, the first borehole dedicated to the study of subsurface life in BULGG was drilled. This presentation will provide an overview of BULGG research activities that are improving our understanding of the physical and chemical controls on the extent and prevalence of subsurface life. Key findings include the influence of electron acceptor availability on microbial diversity, decrease in microbial population sizes with depth and deformation of the host rock, and response of microorganisms to subsurface transport and mixing. The continued development of experiments and this facility by ETH and others will enable us to make more informed predictions about the potential for life on other planets and design missions to explore other subsurface worlds.

# Day 4, Friday, 2.9.2022

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# **904** Investigation of the Faint Young Sun Paradox Through the Lens of Stellar Astrophysical Modeling and Interferometric Observations

KhaDeem D Coumarbatch (1), Petrus Martens (2); William Danchi (3); Vladimir Airapetian (4)

(1) Georgia State University; (2) NASA Goddard Space Flight Center

# **911** The LIFE space mission: characterizing atmospheres of terrestrial exoplanets and searching for habitable worlds and biosignatures

Daniel Angerhausen (1), Sascha Quanz (1), and the LIFE collaboration (2)

(1) ETH Zurich; (2) www.life-space-mission.com

# Talks Session 7

#### 13:00 -13:40

#### **KEYNOTE**

Planetary Atmospheres and the Search for Signs of Life beyond Earth Sara Seager<sup>1</sup> <sup>1</sup>MIT

For thousands of years, inspired by the star-filled dark night sky, people have wondered what lies beyond Earth. Today, the search for signs of life is a key motivator in modern-day planetary exploration. The newly launched James Webb Space telescope will enable us to study gases in rocky exoplanet atmospheres, possibly including "biosignature" gases that might be attributed to life. Closer to home, a now controversial detection of phosphine gas in the Venus atmosphere has reignited studies of Venus, from re-investigation of decades' old atmosphere anomalies to new laboratory investigations of organic molecules' stability and chemistry in sulfuric acid (the composition of Venus' cloud particles). New exoplanet atmosphere discoveries as well as growing evidence for Venus as a potentially habitable planet give us hope towards make progress on answering the ancient questions about the possibility of life beyond Earth.

#### 13:40 - 14:00

#### 37

# Eta Earth Revisited: How many Earth-like Habitats might there be in the Milky Way?

Scherf M<sup>1,2</sup>, Lammer H<sup>1</sup>, Sproß L<sup>2</sup>

<sup>1</sup>Space Research Institute, Austrian Academy of Sciences, <sup>2</sup>Institute of Physics, University of Graz

Without aerobic life, the simultaneous presence of N2 and O2 in the Earth's atmosphere would be chemically incompatible over geologic timescales. The existence of an N2-O2-dominated atmosphere on an exoplanet would, hence, not only constitute a potential biosignature of aerobic life. It would also have to meet certain astro- and geophysical criteria to originate, evolve and to sustain.

Our definition of Eta-Earth, therefore, builds on the concept of a so-called Earth-like Habitat (EH), i.e., a planet within the complex habitable zone for life, at which N2 and O2 are simultaneously present as the dominant species while CO2 only comprises a minor constituent in its atmosphere. By our present scientific knowledge, certain criteria must be fulfilled to allow the existence of such an Earth-like atmosphere. These can be subsumed within a new probabilistic formula for estimating a maximum number of EHs. Some of these criteria, such as the bolometric luminosity and XUV flux evolution of a star, or the distribution of rocky exoplanets within the habitable zones of different stellar spectral types, are already rather well studied and can be tested through further observations. Other important criteria, like the prevalence of working carbonsilicate and nitrogen cycles, or the origin of life are by now poorly, or entirely un-constrained. Further factors, like the presence of a large moon or the importance of an intrinsic magnetic field, are not only poorly constrained but its significance for the evolution and stability of an Earth-like Habitat are even debated. While our new formula for estimating the maximum number of EHs can in principle incorporate all these factors as well as unknowns, we by now must restrict ourselves to the ones that are either well understood or can at least be tested soon. Based on our current knowledge, this approach only allows us to probabilistically estimate a maximum number of exoplanets on which an Earth-like Habitat can in principle evolve. The real number of EHs might, therefore, be significantly lower than our current best estimate but additional criteria should be verifiable in near future by upcoming ground- and space-based instrumentation such as PLATO, the E-ELT, or by the kinds of the proposed space-based observatory LUVOIR.

By considering all the factors that are presently scientifically quantifiable to at least some extent, we will present our current best estimate for the maximum number of EHs that might exist within the galaxy and will particularly focus on the role a star might play in the evolution and stability of such a habitat. If we substitute Eat-Earth, the mean number of rocky planets per star within the habitable zone, to only account for the mean number of EHs per star, Eta-EH, we end up with a number much smaller than the current best estimates for Eta-Earth. It is, therefore, scientifically not justified to presume that all potential habitats inside a habitable zone for complex life will evolve similar to Earth.

#### 14:00 - 14:20

#### 53

#### Detecting super-Earths in the habitable zone

**Hara N<sup>1</sup>**, Dumusque X<sup>1</sup>, Crétignier M<sup>1</sup>, Unger N<sup>1</sup>, Delisle J<sup>1</sup> <sup>1</sup>Université de Genève

Direct imaging is one of the most promising ways to characterize the atmosphere of Earth-like planets and find biosignatures. The yield of the upcoming spectro-imagers such as PCS@ELT, LUVOIR/HaBex is greatly improved if targets are detected in advance. Our goal is to detect terrestrial planets in the habitable zone of their star within 15 pc of the Earth. Radial velocities are capable, in principle, to detect such targets, but are severely limited by the presence of stellar activity. In this talk, I present the recent advances we made in the data analysis of radial velocities, their application to HARPS data, and the detection of new candidates in the habitable zone. This progress opens perspectives on a new census of nearby stars.

# Exploring habitability evolution in rocky planets with climate and atmospheric models

**Silva L<sup>1,2</sup>**, Biasiotti L<sup>3,1</sup>, Bisesi E<sup>1</sup>, Ivanovski S<sup>1</sup>, Maris M<sup>1,2</sup>, Murante G<sup>1,2</sup>, Simonetti P<sup>1,3</sup>, Vladilo G<sup>1</sup> <sup>1</sup>INAF/OATs, <sup>2</sup>IFPU, <sup>3</sup>UniTs

The potential of hosting surface liquid water on rocky planets is generally quantified according to the current stellar and planetary parameters of the detected planets. On the other hand, the potential of currently hosting life rests on environmental conditions favorable for the onset of life at early evolutionary phases. These phases are characterized by lower instellations, and, as for Earth, also a range of different planetary parameters are to be expected (e.g. land-ocean coverage, rotation rate). The ensuing potential evolution of the surface/atmospheric conditions implies different observable transit/emission spectra. We have developed a flexible climate model (ESTM, Earth-like planet Surface Temperature Model, Vladilo et al. 2015; Biasiotti et al. 2022) coupled with a radiative transfer atmospheric model (EOS, Simonetti et al. 2022) for terrestrial-type exoplanets suited for multi-parameter explorations (atmospheric pressure and composition; stellar type; orbital and planetary parameters). Among other applications, we can track the conditions of habitability as a function of the luminosity evolution of the central star, and of other evolving planetary factors.

We have applied our models to investigate the epoch of the onset of life-sustaining conditions in Kepler-452b (Silva et al. 2017), and are exploring the range of atmospheric compositions allowing a habitable Archean Earth. The EOS RT model allows us to compute the expected spectrum for each simulated climate.

References

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# 15:15 -15:35

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### CO2 ocean bistability on terrestrial exoplanets

#### Graham R<sup>1</sup>, Lichtenberg T<sup>1</sup>, Pierrehumbert R<sup>1</sup>

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Cycling of carbon dioxide between the atmosphere and interior of rocky planets can stabilise global climate and enable planetary surface temperatures above freezing over geologic time. However, variations in global carbon budget, tectonics, and unstable feedback cycles between planetary sub-systems have the potential to destabilise the climate and surface geochemistry of rocky exoplanets toward regimes unknown in the modern Solar System.

We performed atmospheric radiative transfer and surface weathering simulations to probe the stability of climate equilibria for rocky, ocean-bearing exoplanets at instellations relevant for planetary systems in the outer regions of the circumstellar habitable zone across different tectonic settings and stellar masses. Characterising these planets with future astronomical surveys will inform our understanding of the diversity of climate states of rocky planets, particularly under low irradiation and with increasing atmospheric carbon budget, similar to the early Earth.

Our simulations suggest bistability between an Earth-like climate state with efficient carbon sequestration and an alternative stable climate equilibrium where CO<sub>2</sub> condenses at the surface and forms a blanket of either clathrate hydrate or liquid CO<sub>2</sub>. At increasing instellation and with ineffective weathering, the latter state oscillates between cool, surface CO<sub>2</sub>-condensing and hot, non-condensing climates. CO<sub>2</sub> bistable climates can emerge immediately upon magma ocean crystallisation and remain stable for billions of years.

The carbon dioxide-condensing climates follow an opposite trend in CO<sub>2</sub> partial pressure versus instellation compared to the weathering-stabilised planet population, with divergent spectroscopic features in the near-to mid-infrared. This suggests the possibility of observational discrimination between these distinct climate categories across the rocky exoplanet census.

# 15:35 – 15:55

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### Biosignatures through rocky planet evolution around other stars

**Rugheimer S<sup>1</sup>**, Kaltenegger L, Rimmer P <sup>1</sup>York University

When we observe the first terrestrial exoplanet atmospheres, we expect to find planets around a wide range of stellar types, UV environments, and geological conditions. Since the first exoplanets available for characterization will be likely for M dwarf host stars, understanding the UV environment of these cool stars is a vital step in understanding the atmospheres of these planets. Additionally, the atmospheres of these planets will not been fixed in time. Earth itself offers many possible atmospheric states of a planet. We set out to examine how an Earth-like planet at different geological epochs might look around FGKM star types from a prebiotic world to modern Earth.

### 15:55 – 16:15

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#### Is ozone a reliable proxy for molecular oxygen?

**Kozakis T<sup>1</sup>**, Mendonça J<sup>1</sup>, Buchhave L<sup>1</sup> <sup>1</sup>Technical University Of Denmark

Molecular oxygen (O2) paired with a reducing gas is regarded as a promising biosignature pair for atmospheric characterization of terrestrial exoplanets. In circumstances when O2 may not be detectable in a planetary atmosphere (for instance, at mid-IR wavelengths) it has been suggested that O3, the photochemical product of O2, could be used as a proxy to infer the presence of O2. While O3 is not directly produced by life, it plays an important role in habitability as the ozone layer is the primary source of UV shielding for surface life on modern Earth. However, O3 production is known to have a nonlinear dependence on O2, as well as being strongly influenced by the UV spectrum of the host star. To evaluate the reliability of O3 as a proxy for O2 we used Atmos, a 1D coupled climate/photochemistry code, to study the O2-O3 relationship for "Earth-like" habitable zone planets around a variety of stellar hosts (G0V-M5V) for O2 abundances from 0.01%-150% of the Present Atmospheric Level (PAL) on modern Earth. We studied how O3 emission features for these planetary atmospheres varied for different O2 and O3 abundances using the radiative transfer code PICASO. Overall we found that the O2-O3 relationship differed significantly around different stellar hosts, with different trends for hotter stars (G0V-K2V) than cooler stars (K5V-M5V). Planets orbiting hotter host stars experience an increase in O3 when O2 levels are initially decreased from the present atmospheric level, with maximum O3 abundance occurring at 25-55% PAL O2. Although this effect may seem counterintuitive, it is due to the pressure dependency on O3 production, as with less atmospheric O2 incoming UV photons capable of O2 photolysis are able to reach lower (denser) regions of the atmosphere to spark O3 formation. This effect is not present for planets orbiting our cooler host stars (K5V-M5V), as the weaker incident UV flux (especially FUV flux) does not allow O3 formation to occur at dense enough regions of the atmosphere such that the faster O3 production outweighs a smaller source of O2 from which to create O3. As a result, for cooler host stars the O3 abundance decreases as O2 decreases, albeit nonlinearly. Interpretation of O3 emission spectral features was found to require knowledge of the atmosphere's temperature profiles -particularly the temperature differences between the planetary surface and stratospheric temperature- which are highly influenced by the amount of stratospheric O3. Planets experiencing higher amounts of incident UV have more efficient O3 production and UV absorption leading to larger stratospheric temperature inversions, and therefore shallower emission features. Overall it will be extremely difficult (or impossible) to infer precise O2 levels from an O3 measurement, however, with information about the UV spectrum of the host star and context clues, O3 will provide valuable information about potential surface habitability of an exoplanet.

### 16:15 - 16:35

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# Looking for biosignatures in exoplanets atmospheres with RISTRETTO and ANDES: a topic at the heart of the newly created Life in Universe Center in Geneva

**Bolmont E<sup>1,2</sup>**, Lovis C<sup>2,1</sup>, Ehrenreich D<sup>1,2</sup>, Kasparian J<sup>1,2</sup>, Ibelings B<sup>1,2</sup>, McGinnis D<sup>1,2</sup>, Winssinger N<sup>1,2</sup>, Caricchi L<sup>1,2</sup>, Castelltort S<sup>1,2</sup>, Mueller A<sup>1,2</sup> <sup>1</sup>Center Life in the Universe, <sup>2</sup>University of Geneva

Since the detection of the first exoplanet orbiting a star like the Sun, the University of Geneva has been at the forefront of exoplanet research. Starting from an extensive expertise in planet detection (with radial velocity), the observatory is also now an important actor in the atmosphere characterization of exoplanets (e.g. Ehrenreich et al. 2020). Today the focus is shifting towards the atmospheric characterization of small temperate planets, such as Proxima-b and the TRAPPIST-1 planets. The university is therefore actively participating to the ground-based instruments RISTRETTO@VLT and ANDES@E-ELT. These instruments will use a technique based on high-contrast imaging and high-resolution spectroscopy to characterize the reflected light from temperate planets and to eventually detect biosignatures in their atmospheres. In particular, it has been shown that such a method could lead to a detection of oxygen in the atmosphere of Proxima-b (Lovis et al. 2017).

However, to be able to correctly identify a biosignature, one needs to be able to identify false positives. So, one needs to know how the atmosphere interacts with the planetary interior, with the incoming stellar radiation, and with many different other processes. A multi-disciplinary approach is therefore necessary.

Recently, and following the 2019 Nobel prize in physics attributed to Michel Mayor and Didier Queloz for the discovery of 51 Peg b, the University of Geneva decided to create a faculty center, the "Life in the Universe Center". The members of the center include experts in astrophysics, geophysics, chemistry, climatology and biology. The center aims at leading interdisciplinary projects on the origin of life on Earth and the search for life in our solar system and in exoplanetary systems to contribute to the world research on fundamental questions: How did life emerge and how did it diversify on Earth? What is the nature of life? Is the Universe full of life? How can we detect life elsewhere than on Earth?

Several projects have started and will start in the near future in the center on the following topics:

- The rise of molecular complexity on primitive Earth
- Multi-stability of climates and habitability
- Evolution under extraterrestrial conditions
- The atmosphere as a mirror for geological processes

I will present some of these new interdisciplinary scientific projects and how they relate to the search of biosignatures in exoplanets atmospheres that we will be able to carry out with instruments like RISTRETTO and ANDES.

# Could the mid-infrared space interferometer LIFE find biosignatures in the spectrum of the Earth in time?

**Alei E<sup>1,2</sup>**, Konrad B<sup>1</sup>, Rugheimer S<sup>3</sup>, Mollière P<sup>4</sup>, Angerhausen D<sup>1</sup>, Quanz S<sup>1,2</sup>, the LIFE collaboration<sup>5</sup> <sup>1</sup>ETH Zurich, Institute for Particle Physics & Astrophysics, <sup>2</sup>National Center of Competence in Research PlanetS (www.nccrplanets.ch), <sup>3</sup>Oxford University, <sup>4</sup>Max-Planck-Institut für Astronomie, <sup>5</sup>The LIFE collaboration (www.life-spacemission.com)

At the dawn of the search for life in the universe, we are focusing our efforts on designing new instruments that are able to characterize the atmospheres of terrestrial exoplanets. One of our main goals is to find "biosignatures", the spectral signatures of gases linked to potential biological activity (e.g. O2 and its photochemical product O3, as well as CH4). Using nulling interferometry in the mid-infrared wavelength range, the Large Interferometer for Exoplanets (LIFE, Quanz et al. 2018, 2021) will allow us to further constrain the bulk parameters and the surface conditions of a few dozens of terrestrial planets, as well as to gather information about their atmospheric structure and composition. At this stage of the mission development, atmospheric retrieval studies are essential to determine the technical requirements for LIFE. Because of the lack of observational data, we rely on theoretical spectra of terrestrial exoplanets to develop analysis pipelines that could be most effective for the characterisation of such targets. We feed these spectra to Bayesian retrieval routines to produce a statistically robust analysis of an atmospheric spectrum given a set of parameters (pressure-temperature structure, chemical abundance, planetary dimensions). In this contribution, we analysed simulated spectra of the Earth at various stages of its evolution calculated by Rugheimer & Kaltenegger (2018): a prebiotic Earth at 3.9 billion years ago (Ga), the Earth after the Great Oxygenation Event (GOE) at 2.0 Ga, and after the Neoproterozoic Oxygenation Event (NOE) at 0.8 Ga, and the modern Earth. We considered an Earth-sized planet on a 1 AU orbit around a Sun-like star at 10 pc from the observer, at the minimum LIFE requirements (spectral resolution R=50, signal-to-noise ratio S/N=10, wavelength range  $\Delta\lambda = 4 - 18.5 \,\mu$ m) as determined in Konrad et al. (2022). We created mock observations with LIFE by running the simulated spectra through the LIFEsim simulator (Dannert et al., 2022) considering all major astrophysical noise sources.

We find that, with the minimum requirements, LIFE could detect O3 in the atmosphere if the O2 abundance is at least 2% (10% Present Atmospheric Level). This corresponds to the NOE and the modern Earth scenarios. CH4 could be constrained in terrestrial atmospheres if its abundance is of the order of 0.1% (GOE and NOE Earth scenarios). We find that the NOE Earth is a particularly convenient scenario to simultaneously constrain O3 and CH4. To retrieve more precise and accurate results of the O3 and CH4 abundance in atmospheres of potentially inhabited exoplanets, we suggest increasing the S/N to 20 for the most promising candidates (Alei et al., 2022).

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# Posters Session 7

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# Reconsidering the habitability of planets in the light of climate multistability

**Bhatnagar S<sup>1</sup>**, Bolmont E<sup>1</sup>, Brunetti M<sup>1</sup>, Kasparian J<sup>1</sup> <sup>1</sup>University of Geneva

The search for life in the universe is one of the major drivers of astrophysics research. Both, external factors (e.g., stellar type) and internal ones (e.g., climate + geophysics) affect the habitability of planets, and consequently, the habitable zone (HZ; Kasting et al. 1993). The climate of a planet is a complex system where different components (the atmosphere, ocean, ice, biomes and so on) interact non-linearly. The core idea of climate multistability is that under the same external forcing, a planet can exist in multiple alternative steady states due to several feedbacks (for e.g., the ice-albedo feedback, Boltzmann radiation, clouds; Strogatz 2018; Brunetti et al. 2019). Multistability can have implications for habitability as planets can shift from an uninhabitable to a habitable state (or vice-versa), at the same external forcing. If these transitions occur very quickly, life might not be able to cope with the change, and could potentially cease to exist. Abrupt climatic transitions have also occurred several times even on Earth, with the climate cycling between temperate and glacial/snowball conditions (Evans et al. 1997; Hoffman et al. 1998). These have been the cause of some mass extinction events and subsequent recoveries of life. In this study, we investigate climate multistability and its implications on habitability and the HZ. We

construct a 1-dimensional energy balance model and implement typical climate feedbacks, including a runaway greenhouse effect parameterisation for high temperatures (>322.5 K; Turbet et al. 2021; Chaverot et al. in prep). With this model, we obtain three steady states for an Earth-like aquaplanet at 1.00 AU from a Sun-like star: (a) Snowball (204 K), (b) Warm State (290 K), and (c) Very Hot State (888 K). We further find that the HZ extends between 0.94 AU to 1.01 AU for this model planet. Moreover, we also show that for a slower-rotating version of this Earth-like aquaplanet, the HZ extends between 0.90 AU to 1.08 AU. Multistability facilitates uninhabitable states (e.g., snowball) to tip into a habitable one (e.g., warm state), potentially extending the range of planets that may have access to a habitable regime. In the near future, these simulations will be refined using a more extensive and robust climate model, the 3-D LMD-Generic Global Climate Model (LMDG GCM).

# Towards Detecting Signatures of Life with the Future LIFE Telescope

**Konrad B<sup>1,2</sup>**, Alei E<sup>1,2</sup>, Angerhausen D<sup>1,2</sup>, Quanz S<sup>1,2</sup>, the LIFE team<sup>3</sup> <sup>1</sup>*ETH Zürich*, <sup>2</sup>*National Center of Competence in Research PlanetS (www.nccr-planets.ch)*, <sup>3</sup>*www.life-space-mission.com* 

Temperate terrestrial exoplanets commonly occur in our galaxy (Bryson et al., 2021). A long-term goal of exoplanet research is to characterize the atmospheres of a sizable sample of temperate planets, and identify habitable or even inhabited worlds. Since the sensitivity of planned telescopes is likely insufficient, we focus our efforts on designing next generation telescopes such as the space-based 'Large Interferometer For Exoplanets' (LIFE, Quanz et al. 2018, 2021). LIFE will measure the mid-infrared (MIR) thermal emission spectrum of exoplanets, which encodes valuable information on the exoplanet's size, atmospheric pressure-temperature structure, and atmospheric composition. One aim is to search for 'biosignature pairs' in these atmospheres. These are pairs of gases that rapidly react with each other and therefore should not be present simultaneously in an exoplanet atmosphere, unless replenished at a high rate by life. An example of such a pair is O2 and its photochemical byproduct O3 together with CH4 or N2O, (Lovelock 1965, Lippincott et al. 1967).

A crucial step in the development of LIFE is to determine how accurately an exoplanet's MIR spectrum needs to be determined in order to be able to robustly infer the presence of biosignature pairs in its atmosphere. To answer this question, we study a simulated Earth-twin exoplanet orbiting a Sun-like star at a distance of 10 pc (Konrad et al. 2021). We use LIFEsim (Dannert & Ottiger et al. 2022) to calculate the wavelength-dependent signal-to-noise ratio (S/N) of the exoplanet spectrum expected for observations with LIFE, and consider all major astrophysical noise sources. We generate a grid of observations covering different wavelength ranges, spectral resolutions (R) and S/Ns. We then use an inverse modeling approach to analyze how well the atmospheric structure and composition of the Earth-twin exoplanet can be constrained from different quality MIR spectra and if the biosignature pairs of interest are detectable. These results provide first constraints for LIFE's instrument requirements.

We find that Earth-like O3 abundances are detected in all simulated LIFE observations, due to the strong O3 MIR absorption feature. Since O3 is a photochemical byproduct of O2, its detection indicates that significant amounts of O2 are present in the atmosphere too. Earth-like N2O abundances are not detectable in any of the considered cases. In contrast, the detection of CH4 shows a strong dependence on the quality of the measured spectrum. For high quality spectra (R of at least 50, S/N of at least 10), we can detect Earth-like CH4 abundances and infer the presence of the O2/O3-CH4 biosignature pair, which could be interpreted as a first indicator of biological activity.

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# Investigation of the Faint Young Sun Paradox Through the Lens of Stellar Astrophysical Modeling and Interferometric Observations

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(1) Georgia State University; (2) NASA Goddard Space Flight Center

The Faint Young Sun Paradox (FYSP) describes a gap in our understanding of the evolution of life as we know it as it implies that liquid water on both Earth and Mars should have been frozen during the early evolution of the Sun. By utilizing the one-dimensional MESA (Modules for Experiments in Stellar Astrophysics) code, we investigate the parameters of an initially more massive Sun at different ages along its main sequence lifetime. A second approach to the same paradox is the observational study of Sun-like stars at an earlier stage in their evolution. This is achieved with interferometric angular diameter measurements of intermediate mass stars within 60 parsecs using the CHARA Array in conjunction with Gaia EDR3 parallaxes to determine their physical diameters for the use in three-dimensional Magnetohydrodynamic simulations. The overall objective is to address the Faint Young Sun Paradox through stellar astrophysics while applying observational measurements to understand the early Solar System and nearby exoplanet habitability.

# The LIFE space mission: characterizing atmospheres of terrestrial exoplanets and searching for habitable worlds and biosignatures

Daniel Angerhausen (1), Sascha Quanz (1), and the LIFE collaboration (2)

(1) ETH Zurich; (2) www.life-space-mission.com

The atmospheric characterization of a significant number of terrestrial planets, including the search for habitable and potentially inhabited planets, is probably the major goal of exoplanetary science and one of the most challenging endeavours in 21st century astrophysics. The Large Interferometer For Exoplanets (LIFE) addresses this challenge by investigating the scientific potential and technological challenges of an ambitious mission employing a formation-flying nulling interferometer in space working at mid-infrared wavelengths. LIFE's observing wavelength range is 4-17.5  $\mu$ m (requirement) / 3-20  $\mu$ m (goal) and the required spectral resolution is 35 (req.) / 50 (goal). The total mission lifetime is anticipated to be 5-6 years (requirement), consisting of a 2.5 year search phase for the detection of hundreds of planets and an up to 3.5 years characterization phase for the detailed investigation of atmospheric diversity and the search for biosignatures. Breakthroughs in our understanding of the exoplanet population as well as significant progress in relevant technologies justify the need, but also the feasibility, for a future mission like LIFE to investigate one of the most fundamental questions of humankind: Are we alone in the Universe?

### How long can cold planets be warm enough for liquid water?

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Potential habitable worlds outside the solar system might be planets that are very different from Earth. Cold super-Earths which retain their primordial, H-He dominated atmosphere could have surfaces that are warm enough to host liquid water. This would be due to the collision induced absorption (CIA) of infra-red light by hydrogen, which increases with pressure. We investigate the existence and duration of this exotic habitat by simulating planets of different core masses, envelope masses and semi-major axes. Evolution models for the host-stars luminosity and the planet's intrinsic heat and radius are incorporated, as well as an atmosphere evaporation model. We find that terrestrial and super-Earth planets with masses of 1 to 10 Earth masses can maintain temperate surface conditions for more than 9 Gyr at radial distances larger than 2 AU. This suggests that a large number of planets in the galaxy could be candidates for habitability and that the concept of planetary habitability should not only be focussed on Earth-analogues.