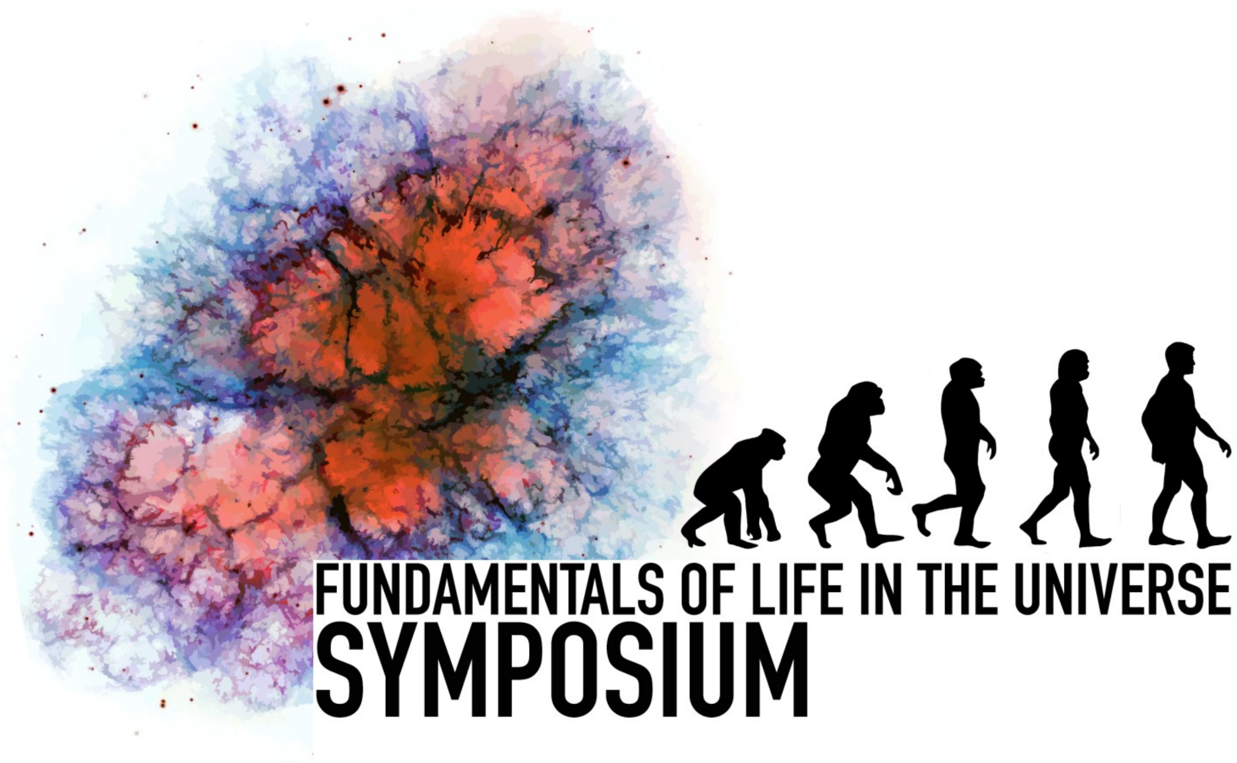

# FUNDAMENTALS OF LIFE IN THE UNIVERSE SYMPOSIUM

August 30- September 1, 2017

Groningen, The Netherlands

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# Introduction

The origin of life, on Earth and elsewhere, is a topic which fascinates the public, and which is ideally suited to bring together scientists from various disciplines. In Summer 2017, we will organize a two-day conference called “Fundamentals of Life in the Universe”, covering a wide spectrum of interests, from planetary evolution to the fabrication of synthetic cells. Besides invited talks, the conference includes a keynote speech by Ben Feringa (2016 Nobel laureate in chemistry), and a public lecture by Charley Lineweaver

**Topics**

1. The origin of the Earth and of life

2. Predicting the evolution of life

3. Building and directing life from molecule to biosphere

4. Life in extraterrestrial environments

5. Emergence and bridging of temporal and spatial scales

## Scientific organizing committee

Matthias Heinemann (GBB, U Groningen)
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Roeland Merks (CWI / U Leiden)
Sijbren Otto (Stratingh, U Groningen)
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Wim Spakman (U Utrecht)
Floris van der Tak (chair; SRON / U Groningen)
Louise Vet (NIOO-KNAW / WUR)
Rens Waters (SRON / U Amsterdam)

## Local organizing committee

Matthias Heinemann
Floris van der Tak
Jan-Willem Mantel
Renate van der Tuuk
Tamara Hummel

# Program

## Thursday, August 31, 2017 Energy Academy

| | |
|---|---|
| 09:00 | Welcome and registration |
| 09:30 | Opening lecture**: John Herlund** (ELSI, Japan)<br>*Copernican inversions in Earth-Life science* |

### Session 1: Origin of the Earth and of life

| | |
|---|---|
| 10:00 | **Geoff Blake** (Caltech, US)<br>*Snow lines in protoplanetary disks and the delivery of volatiles to terrestrial planet surfaces* |
| 10:30 | **Bob Hazen** (Carnegie, US)<br>*Minerals and the origin of life: Insights from big data mineralogy* |
| 11:00 | *Coffee/tea* |
| 11:30 | **John Sutherland** (MRC-LMB Cambridge, UK)<br>*Origins of life systems chemistry* |
| 12:00 | **Paulien Hogeweg** (U Utrecht, NL)<br>*Towards a bioinformatic theory of the origin of life* |

### Session 2: Predicting the evolution of life

| | |
|---|---|
| 12:30 | **Tim Lenton** (U Exeter, UK)<br>*Predicting the evolution of biospheres* |
| 13:00 | *Lunch* |
| 14:00 | **Tetsuya Yomo** (ECNU, CN)<br>*Synthesis and experimental evolution of an artificial cell model* |
| 14:30 | **Marcel Visser** (NIOO-KNAW, NL)<br>*Evolution on a changing planet* |
| 15:00 | **Phil Donoghue** (U Bristol, UK)<br>*The timescale of evolutionary history* |
| 15:30 | *Coffee/tea* |

### Session 3: Building and directing life from molecule to biosphere

| | |
|---|---|
| 16:00 | **Bert Poolman** (U Groningen, NL)<br>*Can we build a minimal form of life from molecular components?* |
| 16:30 | **Cees Dekker** (U Delft, NL)<br>*Divided we stand - from bacterial cell division towards synthetic cells* |
| 17:00 | *Speed networking* |
| 18:00 | *Posters and drinks / "WALKING DINNER" / socializing* |
| 20:00 | **Ben Feringa** (U Groningen, NL)<br>*Designing dynamic molecular systems* |
| 21:00 | *End of day 1* |

## Friday, September 1, 2017 Energy Academy

09:00 **Han Olff** (U Groningen, NL)
*From molecule to biosphere: reductionistic versus emergentistic approaches*
09:30 **Dieter Braun** (LMU, D)
*Recreating the origin of life with non-equilibrium mechanisms?*

### Session 4: Life in extraterrestrial environments

10:00 **Giovanna Tinetti** (UCL,UK)
*Biosignatures in exoplanet atmospheres*

10:30 *Coffee/tea*

11.:00 **Inge Loes ten Kate** (U Utrecht, NL)
*Prospects for life on Mars*
11:30 **Charley Lineweaver** (ANU, Australia)
*What makes planets habitable?*
12:00 **Lee Cronin** (U Glasgow, UK)
*Beyond prebiotic chemistry*

12:30 *Lunch*
13.30 *Poster session*

### Session 5: Emergence and bridging of temporal and spatial scales

14:30 **Peter Sloot** (U Amsterdam, NL)
*The quantum nature of biology and life*
15:00 **Alexander van Oudenaarden** (Hubrecht Institute, NL )
*Whole-organism clone-tracing using single-cell sequencing*
14:00 **Stan Gielen** (NWO, NL)
*The future of research into the origin of life*

16:00 *Coffee/tea*

20:00 **Charley Lineweaver**: *Are we alone in the Universe?*
**Public talk (downtown, Groninger Forum, Hereplein 73, Groningen)**

# Invited Speakers

## Abstracts

# Copernican inversions in Earth-Life science

John Hernlund

Abstract: At the Earth-Life Science Institute (ELSI), based at the Tokyo Institute of Technology, we have been conducting a kind of social experiment for the past 4+ years to understand how we might better rally together Earth/Planetary and Life scientists around big questions such as the origin of life and possibility of life elsewhere in the universe. The idea is quite simple, to assemble a team of talented and open-minded scientists from around the world to form a sort of collective intelligence that is capable of tackling questions that are too big for any one of us to address as individuals. We have been around for a while before ELSI, and we've seen dozens of inter-disciplinary efforts come and go, with mixed success. It was never our intention to repeat the same mistakes we had seen in the past, we had been given a truly remarkable opportunity to do something unique. So, how well have we done thus far? What lessons have we learned, that we might share with others undertaking similar efforts? What is the key to success? I hope that the answers to these questions will surprise you, and perhaps cause you to think differently about approaching the next great national efforts in tackling the grand challenge questions of natural science.

# Snow lines in protoplanetary disks and the delivery of volatiles to terrestrial planet surfaces

Geoffrey A. Blake

*Division of Geological & Planetary Sciences, Caltech*

Compared to the Sun and to the gas+dust composition of the interstellar medium from which the solar system formed, the Carbon and Nitrogen content of the bulk silicate Earth (mantle+hydrosphere+atmosphere) is reduced by several orders of magnitude, relative to Silicon. Evidence from primitive bodies as a function of distance from the Sun suggests that at least part of this depletion must occur early in the process of planetesimal assembly. With pioneering infrared and (sub)mm observations such as those enabled by ground-based 8-10m class telescopes (and in future the James Webb Space Telescope) and the Atacama Large Millimeter Array (ALMA), we can now examine the principal CNO-reservoirs of gas rich disks as a function position within the disk and evolutionary state. Key to these studies is the concept of condensation fronts, or 'snow lines,' in disks - locations at which key volatiles such as water, carbon monoxide, or nitrogen first condense from the gas. This talk will review the observational characterization of snow lines in protoplanetary disks via both gas and dust tracers, especially recent ALMA observations, and highlight the laboratory astrophysics studies and theoretical investigations that are needed to tie the observational results to the delivery of volatiles to planetary surfaces in the habitable zones around Sun-like stars.

# Minerals and the origins of life: Insights from big data mineralogy

Robert M. Hazen (rhazen@ciw.edu)

*Geophysical Laboratory, Carnegie Institution for Science*

Large and growing data resources catalog every known mineral species and their physical, chemical, and structural properties (rruff.info/ima), as well as mineral localities and associations for samples from Earth, the Moon, Mars, and meteorites (mindat.org). These resources are now being linked to deep-time data to facilitate statistical exploration and visual representation of large-scale patterns of mineral diversity and distribution through deep time. Evolution studies of Earth's changing mineralogy through deep time exploit the "Mineral Evolution Database" with more than 120,000 species/locality/age data. These data reveal a dynamic history of mineralization influenced by tectonic and biological processes, including the Wilson cycle, global glaciation, redox changes of the near-surface environment, microbial evolution, biomineralization, and the rise of the terrestrial biosphere.

Origins-of-life researchers have long recognized the plausible roles of minerals in prebiotic chemistry, including molecular catalysis, selection, protection, and assembly. Deep-time data point to several features of Earth's evolving mineralogy that are relevant to these investigations. For example, mineralogical evidence suggests the presence of a relatively limited number of mineral species on Earth at the time of life's origins compared to the more than 5000 species documented today. In addition, data on major and trace element distributions and species diversification confirm other lines of evidence suggesting significant temporal changes in Earth's near-surface oxidation state and, consequently, the distribution of near-surface minerals.

Trends in mineralogical data through deep time are revealed and clarified by use of a variety of visualization methods. Of special note are recent applications of network analysis to investigate complex patterns of mineral coexistence (Morrison et al. 2017; see Figures).

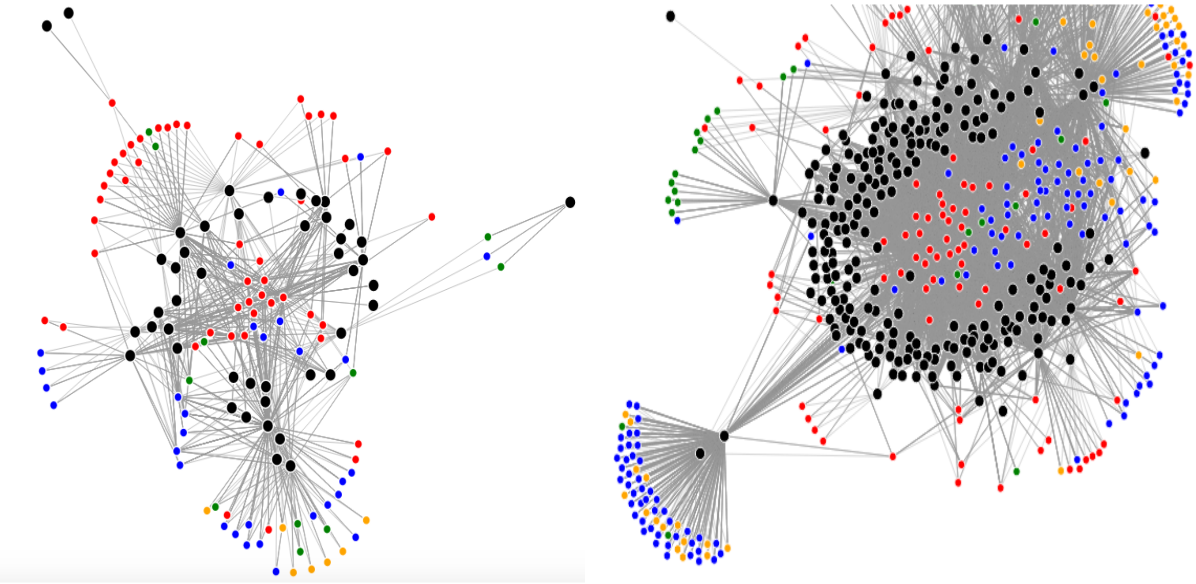

***Figure.*** *Bipartite mineral networks illustrate associations of copper minerals (colored nodes) with major localities (black nodes). Node colors correspond to mineral compositions based on the presence (+) or absence (-) of sulfur and oxygen: red [+S,-O]; orange [+S,+O], green [-S,-O], blue [-S,+O]. Networks for Archean (A) and Cenozoic (B) Cu minerals document a sharp temporal increase in mineral diversity. Distinctive network geometries reveal that relatively few phases are common (i.e., linked to many localities and thus located near the centers of the networks), whereas many more minerals are rare (and thus positioned around the periphery of the black locality nodes). Our work suggests that this frequency distribution may represent a planetary biosignature.*
*[A] Approximately 20 common sulfide minerals dominate the central region of the bipartite network of Archean copper minerals. The periphery has a greater number of rarer, predominantly sulfide and oxides phases.*

*[B] The bipartite network of Cenozoic copper minerals, by contrast, has a much greater diversity of species than observed in Archean rocks. Oxide and sulfate minerals are more prevalent in the Cenozoic compared to the Archean, though a few dozen common sulfide minerals dominate the central region of the network.*

## Reference

*S.M.Morrison et al. (2017) "Mineralogical applications of network analysis." Am. Mineral., in press.*

# Origins of life systems chemistry

John Sutherland

*MRC Laboratory of Molecular Biology, Francis Crick Avenue,*
*Cambridge Biomedical Campus, Cambridge, CB2 0QH, UK*

**Keywords**: Origin of life; prebiotic chemistry; systems chemistry

By reconciling previously conflicting views about the origin of life – in which one or other cellular subsystem precedes, and then 'invents' the others – we suggested a new *modus operandi* for its study. Guided by this, we uncovered a cyanosulfidic protometabolism which uses UV light and the stoichiometric reducing power of hydrogen sulfide to convert hydrogen cyanide, and a couple of other prebiotic feedstock molecules which can be derived therefrom, into nucleic acid, peptide and lipid building blocks [1, 2]. We are now considering the transition of systems from the inanimate to the animate state through intermediate stages of partial 'aliveness', and recent progress in the elaboration of building blocks into larger (oligomeric) molecules and systems in this context will also be described.

## References

*[1] B.H. Patel et al., Nature Chem., 2015, 7, 301-307.*
*[2] J. D. Sutherland, Angew. Chem. Int. Ed., 2016, 55, 104-121.*

# Towards a bioinformatic theory of the origin of life

Paulien Hogeweg

*Theoretical biology and Bioinformatics group*
*Utrecht University*

Living systems as we know them today are complex evolved multilevel information processing systems harboring billions of years of molecular memory (information) in their genome, which is maintained by self-reproduction. This information is processed into a phenotype which may involve an up-scaling of a minimum change at the genome level (one nucleotide substitution) 10 orders of magnitude and yet is robust against noise.

To understand how such systems emerged from 'humble beginnings' is the aim of a bioinformatic theory of the origin and complexi_cation of life

From an evolutionary perspective the RNA world hypothesis is the most commonly evoked as humble beginning", despite sometimes being referred to as "the worst theory of the early evolution of life (except for all the others)".

RNA-like molecules are capable of information storage (the polymer se-quence), as well as information processing (by being a catalyst) in one single molecule,

Here we will review some features of the evolutionary dynamics of RNA-like worlds and discuss the evolution of genotype to phenotype mapping, the emergence of new levels of selection, and the progressive decoupling of information storage and information processing, and therewith the evolution of evolution.

# Predicting the evolution of biospheres

Tim Lenton

*University of Exeter*

Today, nearly four billion years after life first appeared on Earth, the planet hosts an abundance of complex life. The varied and complex life on the planet today both maintains, and is supported by, fertile land and oceans and an oxygen-rich atmosphere, interacting via myriad feedback mechanisms. Furthermore, life and the global environment have co-evolved such that neither would exist in its present form without the other. With a sample size of only one Earth, many have questioned whether the self-regulating of the Earth is just a lucky accident, which had to be that way for us to observe it. However, some basic principles of complex adaptive systems would suggest that it is not an accident and rather that the co-evolution of life and its host planet should tend to converge on self-stabilising attractors. The search for life elsewhere in the solar system and on extrasolar planets should ultimately help us test such theories. In the meantime I will show the results of some experiments *in silico* where we seed many virtual worlds with artificial life forms and see how they evolve. We predict that self-stabilising 'Exo Gaias' should be a frequent though not inevitable outcome wherever simple life forms are able to evolve (or arrive) on a potentially habitable planet. However, the likelihood of such biospheres evolving to a stage of complex, self-aware life, appears far more difficult. Even from our sample of one Earth, it is clear that it only got to its present state of being able to support complex, self-aware life (i.e. us) through a series of highly improbable system-wide 'revolutions', each of which was contingent on the previous one and each of which could have gone catastrophically wrong.

# Synthesis and experimental evolution of an artificial cell model

Tetsuya Yomo

*Institute of Biology and Information Science, ECNU*

The ability to evolve is a key characteristic that distinguishes living things from non-living chemical compounds. The construction of an evolvable cell-like system entirely from non-living molecules has been a major challenge. Here we constructed an evolvable artificial cell model from an assembly of biochemical molecules. The biochemical molecules assembled into micro-scaled lipid vesicles or water-droplets in oil are the artificial genomic RNA, all the molecules required for protein synthesis and RNA replication. In the micro-compartments, the genetic information on the genomic RNA is translated into RNA replicase, which in turn that replicates the original genomic RNA.

After inner replication reaction of RNA, exhausting the nutrient molecules such as nucleic acids and so on, the compartments containing the replicated RNA were subjected to the fusion with other liposomes containing the nutrients and the fission for proliferation in order to get ready for the next RNA replication reaction[1].

Using the translation-coupled RNA replication system, we performed a long-term (600-generation) replication experiment, in which mutations were spontaneously introduced by the translated replicase into its genetic information, and highly replicable mutant RNAs dominated the population according to Darwinian principles. At the beginning of the evolution, the replicated RNA accumulated to form the double strand, a dead-end product for the translation while a small parasitic RNA evolved by a deletion mutation on the original RNA genome to dominate by stealing the replicase translated from the original RNA genome. However, during the evolution, the genomic RNA gradually reinforced its interaction with the translated replicase, thereby acquiring competitiveness against the parasitic RNA. This study provides the first experimental evidence that a simple assembly of biomolecules in a cell-like compartment can autonomously develop their genetic code through Darwinian evolution[2].

## References

[1] *Tsuji G., Fujii S., Sunami T. and Yomo T. (2016) Proceeding of National Academy of Science USA 113(3) 590-595*

[2] *Ichihashi N, Usui K, Kazuta Y, Sunami T, Matsuura T, Yomo T (2013) Nature Communication. 4(2494):1-7 doi :10.1038/ncomms3494.*

# Evolution on a changing planet

Marcel E. Visser[1] & Jacintha Ellers[2]

*[1] Netherlands Institute of Ecology (NIOO-KNAW)*
*[2] VU University Amsterdam*

Evolution has led to a planet that harbours an astonishing biological diversity and variation. Due to climate change, urbanisation and land use change, however, our planet is changing rapidly and species cannot adapt to their changing environment without evolution. Key challenges are how individual phenotypes are shaped by the joint action of genes, genomes and the environment of individuals, and how these phenotypes are selected in natural environments. By joining forces between evolutionary ecologists, genome biologists and earth scientists, we aim to make the transition from understanding to predicting evolutionary change in wild species, essential to forecast the impact of anthropogenic effects on population viability. Ultimately, predicting evolution may enable the development of strategies to steer evolution and apply this knowledge to preserve biodiversity.

# The timescale of evolutionary history

Phil Donoghue

Inferring a unified timescale for the early evolution of Earth and Life is challenging and mired in controversy because of the paucity of surviving fossil evidence, the difficulty of interpreting it, and the challenge of resolving the deepest branches of molecular phylogenetic trees. Surprisingly, it remains perhaps the only episode in evolutionary history where literal interpretations of the fossil record hold sway and, hence, almost every new fossil discovery or reinterpretation leads to a rewriting of evolutionary history. We have attempted to break this cycle using a molecular approach to derive an evolutionary timescale that explicitly incorporates uncertainty associated with fossil sampling, ages, and interpretations. We derive a suite of probabilistic time priors using evidence from palaeontology, sedimentology, isotope geochemistry and the relative timing of endosymbiotic events. Our results are robust to variations parametric variations and the use of different priors. The last universal common ancestor (LUCA) existed soon after the Moon-forming impact, reflecting a rapid transition from prebiotic chemistry to microbial life. Long stem lineages subtend the radiations of the two primary lineages of life: Archebacteria plus Eukaryota and Eubacteria, allowing us to reject the hypothesis that the oldest fossil evidence for life might belong among the living representatives of these groups. The Great Oxidation Event (2.4 Ga) significantly predates the origin of the modern Cyanobacteria (Age), rejecting the hypothesis that photosynthesis evolved in association with the last common ancestor of the extant Cyanobacteria. Eukaryotes emerged very late in Earth history (1.9-1.4 Ga), and we can safely reject the hypothesis that the eukaryote crown radiation was promoted by the Great Oxidation Event. Instead, our results suggest that it was the symbiotic acquisition of the mitochondrion that fuelled the eukaryotic radiation in oceans that were already oxygenic.

# Can we build a minimal form of life from molecular components?

Bert Poolman

*Department of Biochemistry*
*University of Groningen, The Netherlands*

I will focus on the construction of synthetic cells from molecular building blocks rather than the engineering of existing living cells. The systems of this so-called bottom up synthetic biology approach are still relatively simple but they allow a deeper understanding of the molecular processes of the cell, and ultimately reveal what is needed to make the transition from non-life (chemistry; chemical building blocks) to life (“biology”; a system that can sustain itself, grow and divide).

One of the grand challenges in the bottom up assembly of synthetic cells is the construction of functional far-from-equilibrium systems, which are essential in living systems. Here, we report on the functional reconstitution of a pathway for sustained ATP production that performs at least an order of magnitude better than any (equilibrium) system described so far. We maintain energy homeostasis while the load on the system is varied. We use the metabolic energy generation to control the transmembrane fluxes of osmolytes and maintain metabolic activity. We have obtained further understanding of the cell volume regulatory mechanisms in a context and at a level of complexity minimally needed for life.

# Divided we stand - from bacterial cell division towards synthetic cells

Cees Dekker

*Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands*
*c.dekker@tudelft.nl; http://ceesdekkerlab.tudelft.nl*

In my group we use the tools of nanotechnology (nanofabrication, tweezers, fast AFM, fluorescence...) to explore biology at the single-molecule and single-cell scale. Our research ranges from single-molecule biophysics studies of DNA-protein interactions to DNA translocation through solid-state nanopores to exploring biophysics of bacteria with nanofabricated shapes, see http://ceesdekkerlab.tudelft.nl

Recently we have begun a project aimed at realizing synthetic cell division [1]. We study bacterial cell division and work towards building liposomes (lipid vesicles enclosing an aqueous solution with purified proteins and DNA) that can spontaneously divide through a contractile protein ring at the vesicle's perimeter. To realize this, we employ an experimental biophysics approach that addresses both the actual division and the prerequisite spatial control, studying:

(i) Live cell imaging of the FtsZ division machinery. We visualize the movements of cell division proteins in B. subtilis bacteria, and thus discovered that FtsAZ filaments treadmill circumferentially around the division ring, driving the motions of the peptidoglycan synthesizing enzymes that assemble new cell wall of the division site [2]

(ii) Cells in nanofabricated shapes. We study cell-division proteins and DNA in live E.coli bacteria that are molded into user-defined arbitrary shapes and sizes. Clarifying the effects of cell shape will elucidate the guiding principles for the spatiotemporal organization of the cell-division machinery. We can shape live E. coli bacteria into novel shapes such as rectangles, squares, triangles and circles and study spatiotemporal oscillations of Min proteins – associated with cell division – in such artificial geometries of live E. coli cells [3]. We also optically resolve the intrinsic donut topology of the E. coli circular chromosome in shape-manipulated cells, revealing a very dynamic and spatially structured chromosome.

(iii) Proteins and DNA in nanofabricated chambers. We use a bottom up approach to study the basic divisome components in vitro exploiting the full control provided by nanochambers. This approach can resolve the spatial organization of the fascinating patterns of Min proteins [4] and chromatin that dictate the localization of the division ring.

(iv) Liposomes on chip. We have developed a new chip-based technology to generate liposomes for exploring synthetic cell division [5]. We plan to use both microfluidic constrictions and a biomimetic approach (encapsulation of divisome proteins such as FtsZ) to induce liposome splitting, thus enabling a simplified form of synthetic cell division.

## References

*[1] Y. Caspi and C. Dekker, Systems and Synthetic Biology 8, 249-269 (2014).*
*[2] A.W. Bisson-Filho et al, Science 355, 739 (2017)*
*[3] F. Wu, B.G.C. van Schie, J.E. Keymer, C. Dekker, Nature Nanotechn. 10, 719 (2015)*
*[4] Y. Caspi and C. Dekker, eLife doi:10.7554/eLife.19271 (2016).*
*[5] S. Deshpande, Y. Caspi, A. Meijering, C. Dekker, Nature Commun. 7, 10447 (2016)*

# Designing dynamic molecular systems

Ben Feringa

*Stratingh Institute for Chemistry, University of Groningen*
*Nijenborgh 4, 9747 AG Groningen, The Netherlands*

Among the major challenges ahead in the design of complex artificial molecular systems and key to artificial cell like systems is the control over dynamic functions and responsive far-from-equilibrium behaviour. Chemical systems ultimately require control over structure, organization and function of multi-component dynamic molecular assemblies at different hierarchical levels. A major goal is the control over translational and rotary motion.

In this presentation focus is on the dynamics of functional molecular systems as well as triggering and assembly processes. We design switches and motors in which molecular motion is coupled to specific functions. Responsive behaviour will be illustrated in self-assembly and photopharmacology. The design, synthesis and functioning of rotary molecular motors will be presented with a prospect toward future dynamic molecular systems.

Furthermore homochirality of its essential building blocks is a “signature of life”. Approaches and challenges associated with the origin and amplification of chirality are briefly discussed.

## References

*Information on http://www.benferinga.com*
*Molecular Machines: Nature, September 2015*
*Molecular Switches:  Chemistry World, June 2016*

# From molecule to biosphere: reductionistic versus emergentistic appraoches

Han Olff

*University of Groningen*

When trying to understand the origin, development and future of life, we increasingly seek for mechanisms at lower levels of organization; to processes at the level of cells, genes or molecules. Although this reductionist approach has learned us a lot about the components of life, it also has the risk to ignore unique processes that emerge from their interplay at higher levels of organization: complex organisms and ecosystems. In this talk, I explore the emergentistic approach to see how key aspects of organization in living systems arise. In particular, I explore the importance of autocatalysis as an organizational principle. Autocatalytic sets were originally defined in terms of chemical species interacting in biochemical systems where reactions between interacting species catalyze enough substrate for the next reaction so that the whole set of chemical reactions is self-sustaining given sufficient input of energy and essential materials. Such chemical autocatalytic loops, such as the regular and reverse Krebs cycle, are found at the heart of the intermediate metabolism of all organisms, are often statistically and thermodynamically favored over alternative configurations, and may even explain the origin of life. In analogue, I will show how interacting populations of different species in an ecosystem can also form an autocatalytic loop if each species produces the resources needed by the next species in the loop, in such a configuration that the whole set of species is self-promoting and self-sustaining given sufficient input of energy and essential materials (carbon, nutrients). I will argue that autocatalytic processes at the ecosystem level involving autotrophs, herbivores, predators and detritivores are a key component in understanding the origin and subsequent evolution of of life. Without them, nutrients would have come locked up quickly in complex organic compounds limiting further emergence of complexity. In conclude that systems biology should now start to also “look upward” to incorporate organizational principles at the level of ecosystems and earth systems.

# Recreating the origin of life with non-equilibrium mechanisms?

Dieter Braun

*Systems Biophysics, LMU Munich, www.biosystems.physik.lmu.de/, Phone: ++49 89 2180 2317, Fax -16558, Amalienstr. 54, D-80799 München, Germany*

Life as we know it is a stunningly complex non-equilibrium process, keeping its entropy low against the second law of thermodynamics. It is therefore straightforward to argue that first living systems had to start in a natural non-equilibrium setting. We work on a chain of experimental evidence using non-equilibrium microsystems which suggest that geological temperature gradients across porous rock should be able to trigger and drive early molecular evolution. We will report on most recent findings including the explorations of driven phase transitions and replication systems implementing symmetry breaking to locally converge to homogeneous sequence species. We are optimistic to reach the combination of replication and selection of increasingly complex genetic molecules in geologically realistic settings.

# Biosignatures in exoplanet atmospheres

Giovanna Tinetti

*Astrophysics Group, Department of Physics and Astronomy, University College London*

The acquisition of spectroscopic data of the Earth's atmosphere from artificial satellites has changed our perception of terrestrial life and has provided, for the first time, a rigorous scientific framework to search for life elsewhere in our Galaxy. Seen from the outside, our planet appears to be similar, for some aspects, to other planets, yet it shows distinctive signatures of a life-hosting planet, which cannot be found elsewhere in the Solar System.

Lovelock (1965) suggested to search for the presence of compounds in the planet's atmosphere which are incompatible on a longterm basis, i.e. in chemical disequilibrium – for example, oxygen and hydrocarbons co-exist in the Earth's atmosphere. While being the only recipe of biosignature currentlyavailable, is that a robust one?

The discovery of planets around other stars will offer in the next decades the chance to test this hypothesis outside the boundaries of our Solar System. While the number of discovered planets located at the right distance to the star to host some liquid water is increasing by the day, are those objects really habitable or inhabited?

From the little we know about these alien worlds, it appears we need to progress further in the understanding of galactic planetary science before we can commit to a conclusive answer concerning habitability. In this talk I will review the current knowledge about exoplanets and what are, in my view, the necessary steps to be taken in the future to address the question of planetary habitability.

# Prospects for finding Life on Mars

Inge Loes ten Kate

*Department of Earth Sciences -Utrecht University*

Historically, Mars has always been one of the prime targets in the search of extraterrestrial life. This hypothesis was mainly based on its proximity to the Earth and its apparent similarities. Even though Percival Lowell in the very early 1900s announced that he had discovered signs of intelligent life on Mars, follow-up observations only a few years after showed that Mars was a dry, presumably dead planet without any intelligent life. At the dawn of the space era several missions were sent to Mars (Mariners and Vikings), that confirmed the lack of intelligent life and revealed strong evidence for sterile conditions on the Martian surface. More recent observations from telescopes, orbit and ground missions continue to indicate that the current conditions on the Martian surface are too hostile to enable life. There is too little gravity to retain a thick atmosphere, leading to day-night temperature variations in the order of 100 $^{o}$C. There is no magnetic field resulting in the ablation of the upper layers of atmosphere by high energy solar radiation. The composition of this tenuous remnant atmosphere allows for short wavelength ultraviolet radiation to reach the surface. As a result of the low atmospheric pressure, liquid cannot persist on the surface of Mars longer than a few minutes if at all. Given the above, it is worth wondering why Mars is still such a hot topic when it comes to the search for extraterrestrial life?

Over the last 20 years, Mars has become the one of the most studied objects in the Universe, with currently eight active missions investigating a wide range of aspects of our red neighbour. After the Viking mission did not detect life in 1976, these missions have no longer focused on the search for life, but on the identification and characterization of (geo)chemical and (geo)physical processes that shaped the planet and at some stage in its history may have led to conditions favourable for life. These missions have given us an insight in Mars around the time when life appeared on Earth, indicating that the past conditions might have been favourable for microbial life. The focus has now shifted from present to past, but the possibility of life on Mars is still heavily debated.

# What makes planets habitable?

Charley Lineweaver

Exoplanet statistics strongly suggest that rocky Earth-like planets are common and that there is nothing remarkable about the chemical composition of the Earth. The prerequisites and ingredients for life seem to be abundantly available in the Universe. However, we have yet to find any evidence for extraterrestrial life. A common explanation for this is a low probability for the emergence of life (an "emergence bottleneck"), notionally due to the intricacies of the molecular recipe. I will present an alternative Gaian bottleneck explanation (Chopra & Lineweaver 2016): If life emerges on a planet, it only rarely evolves quickly enough to regulate greenhouse gases and albedo, thereby maintaining surface temperatures compatible with liquid water and habitability. Such a Gaian bottleneck suggests that (i) extinction is the cosmic default for most life that has ever emerged on the surfaces of wet rocky planets in the Universe and (ii) rocky planets need to be inhabited to remain habitable. In the Gaian bottleneck model, the maintenance of planetary habitability is a property more associated with an unusual and rapid evolution of biological regulation of surface volatiles than with the luminosity and distance to the host star. During the first billion years of a rocky planets existence there may be no sub-aerial weathering of silicates to produce a negative feedback mechanism for temperature regulation. In the absence of such abiotic negative feedback, a stable circumstellar habitable zone can not exist.

# Beyond prebiotic chemistry

Lee Cronin

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How can matter transition from the nonliving to the living state? The answer is essential for understanding the origin of life on Earth and for identifying promising targets in the search for life on other planets. Most studies have focused on the likely chemistry of RNA, protein, lipid, or metabolic "worlds" and autocatalytic sets, including attempts to make life in the lab. But these efforts may be too narrowly focused on the biochemistry of life as we know it today. A radical rethink is necessary, one that explores not just plausible chemical scenarios but also new physical processes and driving forces. Such investigations could lead to a physical understanding not only of the origin of life but also of life itself, as well as to new tools for designing artificial biology.

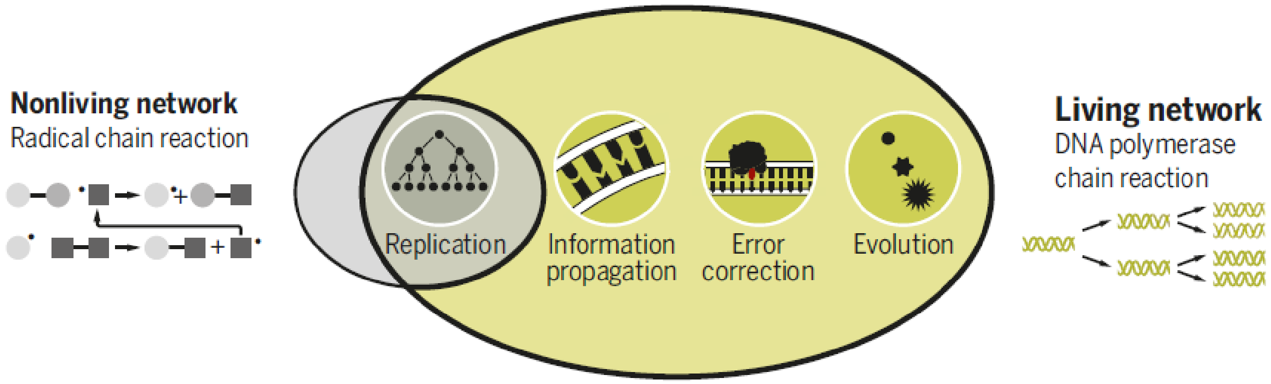

**Figure.** Comparison of nonliving and living networks. Nonliving and living systems both replicate or copy, but the DNA-based living network allows information propagation, evolution, and error correction. Progress in understanding the origin of life may come from studying how simple chemical networks can transform into living networks.

In this talk I will describe our experimental efforts to explore how random chemistry can become less random over time. This is an important question and success may shed light on how complex chemical systems could arise comprising complex molecules, systems and architectures similar to those found in biology today. To do this we have developed a new measure of molecular complexity and have been using this as a new guide, that is chemically agnostic, to discover the simplest pathways that might lead to biology.

# The quantum nature of biology and life

Peter Sloot

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One of the basic questions that Erwin Schrödinger raised in his seminal book '*what is life*' in 1944, was whether the ideas of classical physics, as normally employed by biologists in their understanding of the behaviour of the physical world, are sufficient for explaining the basic features of biology and life. Here we should obviously consider processes like entanglement and (de)coherence that go beyond the basis for the shapes and sizes of biological molecules and their chemical affinities. The sheer spatio-temporal scale on which biology and life operates, across many orders of magnitude, seems to intuitively defy the need for and use of Quantum Mechanics. Yet recent observations and theory indicate that QM might indeed play a role in Biological processes. The question that remains largely unanswered however, is how and to what extend quantum processes drive the up and downward causation in biology. In this talk I will review some of the recent developments of Quantum Biology and reflect on the use of Classical and Quantum Information as a way to reason about causality in biological systems and life.

# Whole-organism clone-tracing using single-cell sequencing

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Whole-organism clone-tracing using single-cell sequencing

Embryonic development is one of the most crucial periods in the life of a multicellular organism. A limited set of embryonic progenitors gives rise to all cells in the adult body. Determining which fate these progenitors acquire in adult tissue is a major challenge and requires the simultaneous measurement of clonal history and cell-type at single-cell resolution. Clonal history has traditionally been quantified by microscopically tracking cells during development, monitoring the heritable expression of genetically encoded fluorescent proteins and, most recently, by utilizing next generation sequencing technology exploiting somatic mutations, transposon tagging, viral barcoding, and CRISPR/Cas9 genome editing strategies. Single-cell transcriptomics on the other hand, provides a powerful technology platform for cell-type classification in an unbiased manner. However, integrating both measurements for many single cells has been a major hurdle. Here, we present ScarTrace, a single-cell sequencing strategy that allows us to simultaneously quantify information on clonal history and cell type for thousands of single cells obtained from different organs from adult zebrafish. Using this approach we show that all blood cells in the kidney marrow arise from a small set of multipotent embryonic progenitors that give rise to all blood cell types. In contrast, we find that cells in the eyes, brain, and caudal tail fin arise from many embryonic progenitors, which are more restricted and produce specific cell types in the adult tissue. Next we use ScarTrace to explore when embryonic cells commit to forming either left or right organs using the eyes and brain as a model system. Lastly we monitor regeneration of the caudal tail fin and identify a subpopulation of resident macrophages that have a clonal origin that is distinct from other blood cell types. We envision that ScarTrace will have major applications in other experimental model systems to match embryonic clonal origin to adult cell-type to ultimately reconstruct how the adult body was build from a single cell.

# The future of research into the origin of life

Stan Gielen

The ambition to understand the origin of life offers many scientific challenges and the results of such an endeavor will have a large impact on our society. However, the roadmap to realize this ambition is not simple. As exemplified by the presentations in this conference, there are many different basic questions in many different research topics that have to be addressed before we can reach a synthesis which might provide insight in the origin of life.

In The Netherlands, both scientists and the general public have contributed to the National Research Agenda. This agenda has 25 routes, which each address an important question or research field. The topic "Fundamentals of Life in the Universe" is one of them. Within each route, researchers with different disciplinary backgrounds will join forces to address the challenges defined by each of the 25 routes. In my presentation I will address possible ways to facilitate research on the National Research Agenda, and in particular research on the topic of "Fundamentals of Life in the Universe". How can we make a serious attempt to work on this theme in The Netherlands. Shouldn't we bring the research topics in these routes as important topics to the European scene? And if so, how can we achieve this ambition in a successful way?

# Are we alone in theUniverse?

Charley Lineweaver

What is humanity doing to try to answer the question ‘Are We Alone?’ and where are we likely to discover life in the near future?

In the last 20 years astronomers have found thousands of planets around other stars. From these discoveries we can infer that every star hosts some kind of planetary system, and that Earth-like planets are common in the universe. However, archaeologists have not found ancient abandoned spacecraft. There is no evidence that we have been visited by technological aliens. And radio astronomers have not found any signals from advanced aliens. Where is everybody? The vast majority of Homo sapiens (including science fiction enthusiasts and professional astronomers) believe that we are not alone. Astrobiologist Charley Lineweaver will discuss the reasons and evidence they give for their opinion, and the evidence that undermines their opinion. What is humanity doing to try to answer the question ‘Are We Alone?’ and where are we likely to discover life in the near future? And what does the word ‘we’ means in the question ‘Are We Alone?’

**Charles H. Lineweaver** is an associate professor and astrobiologist at the Australian National University’s Research School of Astronomy and Astrophysics, and Research School of Earth Science. His astrobiological research involves the origin of the Earth, the origin of life and the origin of cancer. He studies the statistical distribution of exoplanets, the cosmic microwave background radiation, and cosmological prerequisites for the formation of terrestrial planets and life.

**Date**

Friday 1 September 2017 - 8:00 pm to 9:30 pm

**Location**

Groninger Forum, Hereplein 73, Groningen

**Tickets**

Free tickets can be purchased one hour before the lecture at the cash desk of the Groninger Forum

*This lecture is organized in co-operation with the Fundamentals of Life in the Universe Symposium, that is kindly supported by the Royal Netherlands Academy of Sciences (KNAW).*

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AKADEMIE VAN WETENSCHAPPEN

# Poster Abstracts

## (in alphabetical order)

# Conservative evolution: the conditions that spawned life determine and constrain cognition

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**Keywords:** ecology, agency, enactive cognition, wisdom.

Recent work by Smith and Morowitz (2016) addressing the emergence of the biosphere claims that life is a highly efficient biochemical relaxation process of free energy driven by either geochemistry or solar radiation. They propose that life emerged from an ecology of biochemistry and suggest that individuality (agency) is a key to the efficiency of this relaxation process.

This theoretical work connects with insights from enactive cognition, which studies the formal requirements of life, agency, and cognition. New concepts with explanatory power in both domains can be derived by generalizing, reformulating, and reordering key concepts from both knowledge domains while weeding out inconsistencies.

This leads to a central role of two concepts: 'wisdom' as "the ability to (co)create and protect the conditions on which existence depends" and 'power' as "the ability to produce intended results'. These orthogonal abilities span a 2D-plane that emerges at multiple organization levels of life – from life's defining properties to modern societal organization. As such this points to 'conservative evolution'. In addition, these two concepts help to explain why and how Earth self-regulates at states that are not only tolerated by life, but that are actively sustained by activities at the level of the individual.

The work of Smith and Morowitz dovetails with enactive cognition and the synthesis of both domains leads to the formulation of key concepts that have guided the development of life on earth. These are, for that reason, highly relevant to modern humanity.

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# Dynamics of isolated bacterial chromosomes inside synthetic cells

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**Keywords:** Synthetic cells, Nucleoid isolation, DNA organization and dynamics, Microfluidics.

The dynamics and organization of the bacterial chromosome (also: 'nucleoid') are influenced by parameters such as confinement, crowding, supercoiling, nucleoid associated proteins and active processes (e.g. transcription and replication).

It remains unclear to what extent each parameter influences the nucleoid dynamics and structure. To answer this question, we aim to construct an *in vitro* model of the nucleoid. To this end, nucleoids are isolated from cells, cleaned up to obtain bare DNA, labelled and confined inside synthetic cells. These containers confine the nucleoid in one, two or three dimensions (relative to its radius of gyration).

Microfluidics are used to create water-in-oil droplets, which act as the synthetic cells and containers for the isolated nucleoids. These droplets can be captured in traps for observation of DNA dynamics. By changing channel geometry, the initially spherical droplets are forced into tubular or pancake shapes. Using a reservoir in another layer of the microfluidic device, the size of droplets can be varied through the osmosis of water in and out of the droplets.

Labelling specific locations on the DNA enables us to track the movement of that locus as function of the confinement and added proteins or crowding agents. Also, by labelling two loci at variable genomic distances, correlations between these can be explored as function of the aforementioned parameters. In our system, the sequence specific labelling is obtained using a fluorescently tagged dCas9.

Our approach could potentially study the behaviour of two nucleoids inside the same confinement. This system has been modelled in the past by Jun et al. [1], but not experimentally verified. Furthermore, Espeli et al. [2] observed that different genomic loci tend to remain within their distinct areas of the cell. Our approach could elucidate what parameters create these particular dynamics.

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# Engineering of *Escherichia coli* with a hybrid heterochiral membrane

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[#]*Both authors equally contributed to the work*

**Keywords:** lipid biosynthesis, archaeal lipid, LUCA, hybrid membrane

The last common universal ancestor (LUCA) is the most recent organism from which all organisms now living on Earth have a common descent. The membrane composition of LUCA represents an unresolved aspect in the differentiation of Bacteria (Eukarya) and Archaea. The driving force behind this segregation has often been attributed to the chemically instability of a mixed membrane composed by a racemic mixture of Glycerol-1P ether and Glycerol-3P ester based lipids. However, such mixed membranes have never been reproduced in living cells. Here, we present for the first time a stable hybrid heterochiral membrane through lipid engineering of the bacterium *Escherichia coli*. By using a combination of metabolic engineering to boost isoprenoid biosynthesis and heterologous expression of the archaeal ether lipid biosynthetic pathway genes, an *E. coli* strain was obtained with up to 32% of archaeal lipids in the lipidome with the expected chirality. This resulted in viable cells but with altered cell growth, morphology and robustness towards environmental stresses. The hybrid heterochiral membrane bacterial strain sheds new light on the lipid divide and opens novel possibilities for bio-industrial applications.

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# Evolution of novel functions in an RNA-like replicator system

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**Keywords:** evolution, emergence, complexity, RNA world.

How does a prebiotic world with simple replicators evolve the complex set of structures and functions that pave the way for the origin of life? Classical studies on RNA-like replicators indicate that the amount of information that can be accumulated in a genome is severely limited by mutation rates. This seems to hinder the evolution of complexity which relies on the continuous integration of information in genomes.

We show how this problem is overcome in a spatial model of the RNA world. In this model, RNA molecules are endowed with a complex genotype-to-phenotype map, and may replicate each other if their phenotype matches a predefined secondary structure.

We find that a rich ecosystem of novel functions evolves, especially under high mutation rates. These novel functions are fully emergent (i.e. we did not pre-specify them), and are crucial for the survival of the population. The molecules that perform these functions cannot be replicated and only arise from mutations of viable replicators. Among these replicators, we identify a master sequence that encodes the information for the entire ecosystem. High mutation rates are thus exploited by the master sequence to generate functional mutant offspring, which aid its survival.

In conclusion, we show how information can be integrated and maintained under high mutation rates, namely through the evolution of individually-coded but ecosystem-based diversity.

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# Determining temporal changes in Earth's Deep carbon cycle using dated growth zones in individual diamonds

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**Keywords:** diamond, carbon cycle, Earth evolution.

Earth's carbon cycle is the fundamental control on the origin and evolution of life and today is controlled by plate tectonics. Unfortunately Earth's early geological record is poorly preserved and access to the Earth's deep interior, the host of most carbon, limited. The antiquity of some diamonds and their inclusions (> 3.5 Ga) makes them unique probes of Earth's deep interior and potential recorders of temporal changes in C fluxes. Diamonds, however, often record a multi-stage growth history such that dating bulk samples could yield erroneous ages. A new methodology was developed to date individual silicate inclusions (> 40 µm). C-N isotope ratios of host diamond growth zones are also determined.

Successful dating of both peridotitic and eclogitic diamonds is reported. A previously reported age of diamond formation of 2.3 ± 0.04 Ga from Venetia (South Africa) on pooled inclusions is shown to represent two distinct events: (1) Archaean diamonds formed by relatively cool fluid-dominated metasomatism at 2.95 Ga; and (2) Proterozoic diamonds formed almost two billion years later (1.15 Ga) by melt-dominated metasomatism related to large-scale regional magmatism. Eclogitic diamonds from Botswanan mines record multiple (n>6) diamond growth events. Individual diamonds have growth zones up to 2 Gyr different in age. The distinct diamond forming events involved carbon derived from at least 3 different sources, interpreted as the asthenosphere and recycled organic-rich and carbonate-rich sediments, the involvement of which vary with time.

The success of these studies allows the possibility for systematic study of the temporal changes in carbon and nitrogen isotopes in diamonds to quantify the evolution of Earth's volatile element cycles. To fully interpret the implications of such data requires integrated studies that consider the tectonic, physical and chemical properties of subduction zones; the region of the Earth where tectonic plates recycle volatiles into the Earth's interior.

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# Building the habitability ladder: from the Milky Way to cosmological scales

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Keywords: Astrobiology, Milky Way, Local Universe, cosmological simulations

I will present the first model (Forgan et al. 2017) that couples high-resolution simulations of the formation of Local Group galaxies with calculations of the galactic habitable zone (GHZ), a region of space which has sufficient metallicity to form terrestrial planets without being subject to hazardous radiation. These simulations allow us to make substantial progress in mapping out the asymmetric three-dimensional GHZ and its time evolution for the Milky Way (MW) and Triangulum (M33) galaxies, as opposed to works that generally assume an azimuthally symmetric GHZ. We show that while a large number of habitable planets exist as close as a few kiloparsecs from the galactic centre, the probability of individual planetary systems being habitable rises as one approaches the edge of the stellar disc. Tidal streams and satellite galaxies also appear to be fertile grounds for habitable planet formation.

I will then extend this framework to the entire local Universe (Dayal et al. 2015) to answer the tantalising question: Which type of galaxy is most suitable for hosting life in the cosmos? In an exciting development, the three key astrophysical criterion governing habitability (total mass in stars, total metal mass and ongoing star formation rate) are found to be intricately linked through a "fundamental relation" as shown by observations of more than a hundred thousand galaxies in the local Universe. Using this relation we show that metal-rich, star-formation impoverished, shapeless giant elliptical galaxies at least twice as massive as the Milky Way can potentially host ten thousand times as many habitable planets, making them the most probable "cradles of life" in the Universe. Finally, I use this understanding to study the habitability of the entire Universe through 13 billion years of cosmic time, since its inception, till the present day (Dayal et al. 2016).

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*3 Evaluating galactic habitability using high-resolution cosmological simulations of galaxy formation, Forgan et al., 2017, IJAsB, 16, 60*

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# Rapid adaptation of herbivore consumers to nutrient limitation: eco-evolutionary feedbacks to population demography and resource control

Declerck, S.A.J., A. Malo, S. Diehl, D. Waasdorp, K. Lemmen, K. Proios, and S. Papakostas.

Humans alter biogeochemical cycles of essential elements such as phosphorus (P). Prediction of ecosystem consequences of altered elemental cycles requires integration of ecology, evolutionary biology and the framework of ecological stoichiometry. Using an experimental evolution approach we studied micro-evolutionary responses of a herbivorous rotifer to P- limited food and the potential consequences for its population demography and for ecosystem properties. We subjected field-derived, replicate rotifer populations to P-deficient and P-replete algal food, and studied adaptation in common garden transplant experiments after 103 and 209 days of selection. When fed P-limited food, populations with a P-limitation selection history suffered 37% lower mortality, reached twice the steady state biomass, and reduced algae by 40% compared to populations with a P-replete selection history. Adaptation involved no change in rotifer elemental composition but reduced investment in sex. This study demonstrates potentially strong eco-evolutionary feedbacks from shifting elemental balances to ecosystem properties, including grazing pressure and the ratio of grazer:producer biomass.

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# Volatile supply and C/O ratios of planet-building material. The effect of chemical processing in planet birth places

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**Keywords:** Kinetic chemistry, volatile supply, planets

Connecting the observed composition of exoplanets to their formation sites often involves comparing the atmospheric C/O ratio to a disk model with a fixed chemical composition which defines icelines of the dominant volatile molecules (e.g., CO, $H_2O$, and $CO_2$). In this scenario full inheritance of interstellar ices is assumed and chemistry during the planet formation era is not considered. However, kinetic chemical evolution during the lifetime of the gaseous disk can change the relative abundances of volatile species, thus altering the C/O ratios of planetary building blocks. In this talk, new results of chemical evolution models of disk midplanes will be presented. These evolution models utilize a large network of gas-phase, grain-surface and gas-grain interaction reactions, thus providing a comprehensive treatment of chemistry. The results that will be presented show that chemistry does alter the volatile composition of the material in the midplane, as well as the C/O ratios of gas and ice during the epoch of planet(esimal) formation. Thereby, the picture of C/O ratios in disk midplanes defined simply by volatile ice lines in a midplane of fixed chemical composition, is modified. Hence, these results point to the importance of considering chemical evolution in disk midplanes when contrasting observed atmospheric compositions of (exo)planets to their formation locations.

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# Growing membranes: *In vitro* construction of a phospholipid membrane

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**Keywords:** Synthetic cell, Phospholipid biosynthesis, Growing membranes

The construction of a synthetic minimal cell via bottom-up approaches requires the assembly of a minimum number of cellular components (nucleic acids, enzymes, lipids, etc.), that together are capable of executing basal cellular functions. One of the key features defining a cell as a living entity is its ability to self-reproduce. In this process, expansion of the phospholipid membrane barrier is a critical aspect. Here, we engineered an entire phospholipid biosynthesis pathway (Fig.1) existing of a composite of catabolic and anabolic enzymes. The system is based on a cascade of eight purified (membrane) proteins reconstituted into pre-existing liposomes, that are needed as a platform for phospholipid biosynthesis. It starts with simple building blocks such as fatty acids and glycerol-3-phosphate to finally yield the two essential phospholipids phosphatidyl- ethanolamine (PE) and phosphatidylglycerol (PG). This versatile system is capable of converting mixtures of fatty acids into phospholipids with diverse acyl-chain configurations and saturation profiles, as well as simultaneously synthesizing PE and PG, thereby mimicking the phospholipid composition of a biological membrane. Membrane growth was visualized by a combination of Mass Spectrometry and Electron Microscopy, while expansion was quantitated by means of a fluorescent quenching assay that records the density of a fluorescent lipid in the expanded membrane. The observed expansion was as expected and only limited by depletion of fatty acids.

Overall, we report the development of an efficient and versatile system to generate a wide variety of phospholipids from simple fatty acids, thereby growing membranes in a test tube.

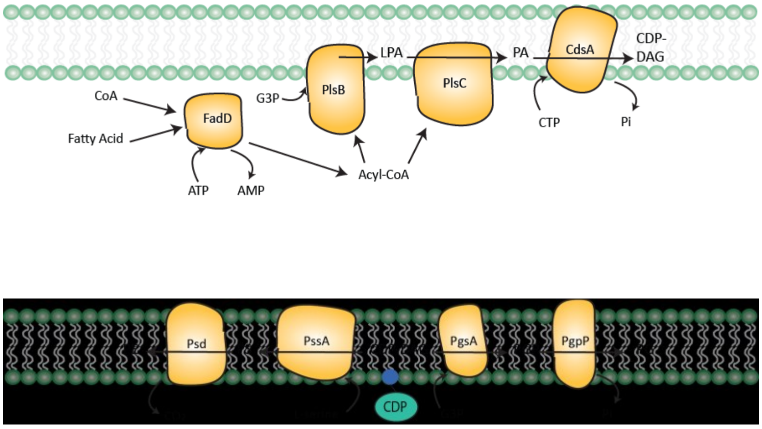

*Fig.1 Schematic representation of the phospholipid biosynthesis pathway*

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# Delivery of organics to Mars through asteroid and comet impacts

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**Keywords:** asteroids, comets, dynamics, Mars

The recent discovery of methane in the Mars atmosphere and organic molecules in drill samples[1] taken by Curiosity is surprising, as photodissociation and photodegradation would destroy most organics within hours. While burying in the subsurface will increase the lifetime, it is clear that organics must have been delivered in geologically recent times, presumably by impacts of asteroids, comets, and/or interplanetary dust particles (IDPs).

The IDP-borne flux on Mars was calculated to be $12 \bullet 10^6$ kg/yr by Flynn[2]. We calculate for the first time the flux from asteroids and comets.

We have performed numerical gravity simulations of impact rates on Mars within the past few Myr. We use the N-body integrator RMVS/Swifter to propagate the Sun and the eight planets from their current positions. Separately, we add comets and asteroids to the simulations as massless test particles, based on their current orbital distributions. In our asteroid simulations we focus on organic-rich (C-class), basing ourselves on the dynamical model by Bottke et al. [3] and on the measured distribution of taxonomic types across the Main Asteroid Belt[4]. For the comets we assume a constant organic fraction.

We estimate the organic flux to be ~$0.05 \bullet 10^6$ kg/yr for asteroids, and ~$0.0002 \bullet 10^6$ kg/yr for comets. We conclude that comets can be neglected in the process of organic delivery to Mars. While IDPs appear to dominate the overall organic delivery, C-type asteroids are probably a non-negligible source of organics on Mars locally, in the areas of impacts.

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# Evolution explains the universality and simplicity of microbial metabolism

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**Keywords:** microbial fitness-optimisation, resource allocation, metabolic-principles.

Many evolutionary distant microbial species show highly similar metabolic behaviour[1], such as overflow metabolism, diauxic growth and catabolite repression, and mixed substrate usage. Overflow metabolism is also shown by autonomously proliferating higher eukaryotic cells, such as cancer cells (known as the Warburg effect). This raises the question whether and how natural selection drives cells towards those common metabolic strategies. We identify an evolutionary extremum principle that determines metabolic behaviour under growth-promoting conditions: fitness maximisation requires minimisation of metabolic complexity. The principle is a mathematical consequence of maximising metabolic fluxes under (enzymatic) constraints. We prove that the number of active constraints determines the number of active minimal metabolic pathways (Elementary Flux Modes) that carry flux in the optimal solution. These constraints are low in number and universal across species, which explains why different species display common fitness effects of protein expression and similar metabolic behaviour. The theory is used to derive three necessary conditions for a micro-organism to show a mixed strategy. The fundamental principle is presented as a (graphical) mathematical framework that provides a deeper, unifying understanding of (mixed) metabolic strategies. We use it to re-interpret experimental results[2] on overflow metabolism and the co-consumption of substrates, demonstrating that the theory has important operational use in the interpretation and design of experiments that can identify the most likely active constraints.

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# Top-down or bottom-up? Towards the construction of a minimal cell division apparatus

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**Keywords:** cell division, cell organization, protein localization

One of the ultimate aims in synthetic biology is the construction of a minimal cell. Importantly, such endeavor will also reveal whether we truly know and understand the basic biological systems that make up a living cell. In essence, there are two approaches, one that tries to build a synthetic cell from simple building blocks, the 'bottom-up' approach, and one that starts with a simple (bacterial) cell and tries to remove non-essential proteins to come to a minimal cell system, the 'top-down' approach. Here we focus on cell division and the spatial organization of proteins in a minimal cell. Since we still do not really know how cell division works in bacteria, we chose the 'top-down' approach and tried to determine what set of proteins are minimally required for bacterial cell division. For the construction of a simplified cell division machinery, we chose the Gram-positive model system Bacillus subtilis. Surprisingly, we were able to remove eight conserved cell division proteins without affecting viability. In the process, we discovered a new cell division influencing protein. This work shows that bacterial cell division is a rather robust process, but it also revealed that it is integrated into other bacterial processes, which should be taken into account when constructing a minimal cell, be it top-down or bottom-up.

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# Putting metabolism on the road: the case for the emergence of life in hot acid

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**Keywords:** Thermoacidophiles, pH disequilibria, chemolithoautrophy, origin of life

There is widespread, but not unanimous, agreement that life emerged in hot, anaerobic conditions by exploiting redox and pH disequilibria found on early earth[1]. Although several hypotheses explain the nature and extent of the postulated disequilibria, few consider that life evolved at very low pH (<3). Such environments are thought to be hostile to life and certainly a poor area to search for clues for the abiotic to biotic transition and the early evolution of energetic pathways. However, low pH environments offer some remarkable opportunities for early biological evolution.

This poster evaluates the pros and cons of the early evolution of life in thermo-acidic conditions. Such environments are thought to have been abundant on early earth and were probably rich in hydrogen and soluble metals including iron and sulfur that could have served as sources and sinks of electrons.

Modern-day thermo-acidophiles thrive in such conditions, displaying a wide range of energetic mechanisms, including chemolithoautotrophy on Fe-S mineral surfaces. Low pH environments are rich in protons that are the major drivers of energy conservation by coupling to phosphorylation in all organisms on earth and this may be a "biochemical fossil" reflecting the use of protons in primitive energy conservation. It has also been proposed that acidic conditions favored the evolution of an RNA world[2].

On the other hand, the idea that life emerged at low pH can be challenged because of the proposed difficulties of folding and stabilizing proteins exposed simultaneously to high temperature and low pH[3]. In addition, although thermo-acidophiles root to the base of the phylogenetic tree of life, consistent with the proposition that they evolved early, yet there are problems of interpretation of their subsequent evolution that must be reconciled with their phylogeny. We propose solutions to these problems, advancing the idea that life evolved in thermo-acidic conditions.

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# Life on a dry planet

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**Keywords:** water, planet formation, plate tectonics

Since water is essential for life as we know it, there has been much emphasis placed on identifying the presence of water on other planetary bodies. This concept has been extended to suggest planetary processes, such as plate tectonics, also require water. Since the surface of our planet is water rich, it is tempting to think of it as a “wet” planet. While most bodies with water lie in the outer solar system beyond the ice line, our Earth is relatively dry by comparison, yet supports both life and plate tectonics. If we were able to examine our solar system from afar, what criteria would allow us to conclude that the Earth is the most likely (in some sense) to harbor life? Since terrestrial planetary formation involves a significant amount of volatile loss, we seek to put some bounds on how dry a planet can be and still potentially support a global biosphere. Many factors contribute to this issue including: incoming solar radiation, solar system mixing, planet size, planet bulk composition, volatile loss, volatile delivery, impact history, atmosphere-magma ocean interactions, core formation, volatile storage capacity, just to name a few. While a complete solution to this issue is beyond the scope of a single study, here we emphasize the importance of the water cycle rather than the water concentration. We characterize the water cycle potential for bodies in our solar system as a first step toward understanding how we might identify the water cycle potential in worlds beyond.

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# Mimicking the interface between influenza and a cell: Bridging molecular and colloidal length and time scales by multivalency

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**Keywords:** molecular recognition, multivalency, bridging length and time scales, artificial cell mimics

Multivalency is the phenomenon that describes the interaction between multivalent receptors and multivalent ligands. It plays a pivotal role in biochemistry, particularly in protein-carbohydrate interactions, e.g., in the infection of cells by the attachment of viruses or bacteria to cell membranes.[1-3] However, multivalency is often poorly understood in a quantitative sense as well as how the dynamics of a system depends on it.[4]

A key point of the current presentation will be how multivalent interactions bridge the length and time scales from individual molecular components to whole viruses and cells. Artificial systems are designed to study the interaction between influenza and a cell surface, which provide a deeper understanding of this interaction. A particular focus is how the dynamics of the individual interactions and their multivalent nature govern the dynamics of the overall system.

We employ self-assembled monolayers using carbohydrates to mimic the cell surface. Virus particles with hemagglutinin are used to study the interaction with the carbohydrate monolayers. Because of the molecular control over both the surface and the particle, the molecular dimensions and the valency of the interaction can be estimated. This allows quantitative interpretation of the affinity, leading to values for the intrinsic binding affinity and the effective molarity. Overall, thermodynamic models confirm the binding between the virus particles and the surface to be weakly multivalent and thus remain dynamic.

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# Predicting lifespan: Death as a tipping point in *C. elegans*

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**Keywords:** Lifespan predictions, *C. elegans*, Tipping point

Aging is a multifactorial, complex trait resulting from a vast network of interacting genetic and environmental processes. In model organisms, aging is often studied in a reductionist approach focusing on single genes to identify key-players of aging. While this approach has been instrumental to identify several central processes, such as the cellular stress response[1], its power to predict lifespan in natural populations is limited.

Considering the complex nature of aging, we propose to complement the reductionist approach with a more system-oriented approach. The paradigm of catastrophic regime shifts has been applied to study the collapse of complex dynamic systems in many disciplines ranging from ecology, sociology to climatology.[2] We hypothesize that the aging process in the model organism *C. elegans* follows the common characteristics of a complex system with death as the result of a tipping point of collapse. Moreover, the paradigm describes early warning signals that predict the occurrence of a system collapse, such as the slowing down of the recovery rate from transient perturbations as the system approaches a tipping point.[3]

We introduce the concept of using *C. elegans* stress response in combination with the paradigm of catastrophic regime shifts to study aging as a complex trait with the ultimate aim of predicting death. We show that during stress exposure, *C. elegans* mounts a highly dynamic response involving the expression of hundreds of genes ending at a point of no return leading to death.[4] We developed a quantitative method that summarizes this vast, and complex transcriptional stress response. Using this method, we analysed the gene expression of 78 genetically diverse strains during heat shock and after a period of recovery. Our data shows that the ability of different strains to recover from heat-shock is predictive of the effect of stress on their lifespan.

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# Phyllosilicates in the young Solar Nebula: Links to asteroids and Earth oceans

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**Keywords:** Protoplanetary Disk; Solar System; Phyllosilicates; Molecular Dynamics.

Endogenous or exogenous, dry or wet, various scenarios have been so far depicted for the origin of water on our Solar Systems rocky bodies. Hydrated silicates found in meteorites and in interplanetary dust particles together with observations of abundant water reservoirs in the habitable zone of protoplanetary disks are evidences that support aqueous alteration of silicate dust grains by water vapor condensation in a nebular setting.

We show here the results of our investigation of the thermodynamics (temperature and pressure dependencies) and kinetics (adsorption rates and energies, surface diffusion etc.) of the hydration reactions of forsterite surface grains, constraining the location in the solar nebula where aqueous alteration by water vapor adsorption could occur efficiently. Our results show that water can efficiently adsorb on dust for warm surface temperatures (300-700K) but that for higher temperatures, water could diffuse within the dust to form phyllosilicates. These two processes provide water reservoirs located at different places in the solar nebula. The adsorbed water could further react on the warm grain surfaces to form phyllosilicates. The products of these processes could be subsequently incorporated into asteroids. Typical percentages of phyllosilicates found in meteorite samples are within the range produced by warm surface chemistry of small grains. The same process could then have contributed to the amount of water in Earth oceans through later outgassing of phyllosilicates from the Earth mantle. The results will appear in two publications: D'Angelo et al. (in preparation) describes the Molecular Dynamics simulations characterizing the efficiency of water adsorption on warm (300-800 K) silicate surfaces under the pressure conditions of the young Solar Nebula and Thi et al. (in preparation) the application in protoplanetary disk models quantifying the phyllosilicate formation through warm surface reactions.

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# Understanding chemical complexity in protostellar outflows: L1157-B1 star forming region

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**Keywords:** astrochemistry, star formation, outflows, shocks, COMs

During the early evolutionary stages of star formation, molecular outflows are produced by the shocked interaction between high-velocity jets driven by the protostar and the ambient material. Shocks quickly release the content of interstellar ices into the gas phase through ice sputtering and trigger a rich endothermic gas phase chemistry. Spatially resolved molecular outflows are known to be chemically rich with the detection of several dozens of species, and provide us a laboratory to test different chemical scenarios. Complex Organic Molecules (COMs), molecules based on carbon chemistry and probably at the origin of the prebiotic chemistry we see in our Solar System, have been routinely detected around protostars in large quantities. The presence of many COMs in star forming regions has been understood as due to warm surface chemistry triggered by UV photolysis. The recent detection of several COMs towards the protostellar outflow prototype L1157-B1 challenges our current understanding of the chemistry producing these COMs[1,2]. The large distance of the shocked source with respect to the central heating protostar suggests that the pre-shock material is too cold to efficiently produce COMs through warm surface chemistry. In this project, we theoretically studied the formation and evolution of COMs occurring in molecular outflows. For this purpose, the results of a state-of-the-art 1D physical shock model[3] were applied into a gas-grain astrochemical model[4] in order to assess whether COMs can be produced in molecular outflows through gas phase chemistry. Then, the results of the model predictions were compared with recent observations carried out with IRAM 30m telescope of the prototype outflow L1157-B1[5]. It is concluded that dimethyl ether (DME) and methyl formate (MF), the two COMs prototypes could be produced in significant quantities in shock regions.

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# The Boltzmann Genome. A self-consistent theory of transcription initiation

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**Keywords:** Transcription initiation, Statistical mechanics, Transcription factors,

In living cells, the proteins associated with gene regulation, the so-called transcription factors, are often shared between multiple pathways simultaneously. Genes therefore have to compete for transcription factors whose availability may fluctuate. Moreover, multiple copies of identical genes may exist in cells. We have developed a self-consistent model for gene regulation suitable for complex regulatory architectures and shared transcription-factors[1]. It will be shown that the competitive effects of the regulatory environment can be isolated into a single effective concentration, allowing the accurate description of a collection of gene expression data from diverse regulatory situations.

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# The importance of cosmic ices for the exogeneous delivery of organic matter onto telluric planets

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**Keywords:** astrochemistry, astrobiology, prebiotic chemistry

Ices made of simple molecules are ubiquitously detected in the infrared spectra of many astrophysical environments such as molecular clouds [1,2] out of which stars and planetary systems do form, together with many icy debris (asteroids, comets, dust…). Ices may also undergo efficient energetic processing, including ultraviolet irradiation at the turbulent edges of protoplanetary disks [3]. Such icy materials can be straightforwardly simulated in laboratory non-directed experiments in which the photo and thermal evolution of these ices are performed using, in our case, vacuum ultraviolet irradiation, following the classical methods of "matrix isolation techniques" [4]. These laboratory ices may then be used as templates for the astrophysical ones, where a complex radical chemistry develops, leading to the formation of a complex organic matter, soluble (in water and classical organic solvents) and insoluble [5], similar to what is indeed observed in primitive carbonaceous chondritic meteorites and known as SOM and IOM. More specific molecules such as amino acids [6] sugars [7,8] and even nucleobases [9] make these materials particularly attractive for the possible onset of a "true" prebiotic evolution at the surface of a telluric planet if adequate conditions are met (mostly liquid water, organic chemistry, free energy…). Global analytical methods using very high resolution mass spectrometry of the soluble organic residues [10,11] reveal the exreme complexity of these organic materials which parallels the one observed in the Murchison chondrite for example [12] or within the Paris meteorite, as far as specific "biological molecular bricks" are considered [13].

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# The square lilometer array and the cradle of life

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**Keywords:** provide four keywords separated by commas.

We provide an overview of the exciting capabilities of the Square Kilometer Array (SKA) in the Cradle of Life theme, as detailed in [1]. With the deployment of the high frequency band 5 receivers, the phase 1 of the SKA can conduct headline science in the study of the earliest stages of grain growth in proto-planetary disks. SKA1-MID can map the 2 cm continuum emission at a resolution of 4 au in the nearest systems and therefore begin to probe the distribution of cm-sized particles across the snow line. This frequency range will also enable deep searches for pre-biotic molecules such as amino acids from pre-stellar cores to the cold, outer regions of proto-planetary disks where cometary material forms. The lowest frequency capabilities of SKA1 can be used to examine the magnetic fields of exo-planets via their auroral radio emission. This gives unique insight into their interiors and could potentially detect exo-moons. Across the full frequency range, the SKA1 will also carry out systematic, volume-limited searches of exo-planet systems for signals from technologically advanced civilizations. The sensitivity of SKA1 means that these only need to be at the level of typical airport radar signals in the nearest systems. Hence, the SKA1 can conduct high impact science from the first steps on the road to planets and life, through areas affecting the habitability of planets, and ultimately, to whether we are alone in the Galaxy. These inspirational themes will greatly help in the effort of understand the origins and prevalence of life in the Universe.

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# Using evolutionary biology to study group selection in chemistry

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**Keywords:** Composomes, Evolution, Cooperation, Population dynamics

A biological cell is a highly complex and coordinated system of molecular interactions. Its constituents (DNA, RNA, proteins and smaller molecules) operate together to perform tasks, perhaps the pinnacle of which is the cell's replication. This stands in contrast to known abiotic chemical systems, which, although can be messy and complex, seem not to exhibit the cooperative and coordinated nature of a cell’s molecular processes. Here, we postulate that selection at the molecular level can be a driving force for complexification in chemical systems, in particular during the origins of life and prior to the emergence of biological replication, and we propose to study the emergence of cooperation between molecular processes based on that assumption.

In the biological theory of multilevel selection there are two selective forces: within-group selection which tends to favor 'selfish' replication of individuals, and between-group selection which can favor cooperation between individuals enhancing the fitness of the group as a whole. These forces can be quantified using the multilevel Price equation1, a standard tool used in evolutionary biology to quantify evolutionary change2. Cooperation can only emerge when between-group selection outweighs within-group selection.

We demonstrate this using the established Graded Autocatalysis Replication Domain (GARD) model3, describing simple protocells composed out of molecules with their replication triggered by growth and split. A protocell and its molecular constituents respectively analog to the group and the individuals. Our goal is to demonstrate how molecular cooperation arises in this system as a result of group selection which leads to between-protocells selection being higher than the average within-protocells selection.

Furthermore, by doing so we propose an analogy between the biological relation of parent-progeny to the reactant-product relation in chemistry. This would allow for tools from evolutionary biology to be applied to chemistry and would further deepen the connection between chemistry and biology.

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# PEPSci - The planetary and exoplanetary science programme

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**Keywords:** exoplanets, planetary science, astronomy, geosciences

The Dutch Planetary and ExoPlanetary Science programme (PEPSci) is an initiative of NWO to establish a coherent and integrated network on the interface of astronomy and earth sciences. The programme focuses on the characterisation of planetary processes both within our own solar system and on exoplanets. The addressed topics span the full range from observations and modelling of planetary formation, planetary structures, geology, and atmospheres to the investigation of chemical and biological processes that are linked to organic matter and life. Eight projects have been granted in PEPSci, aimed at understanding the origin, structure and evolution of rocky planets and at identifying the best approaches to detect biosignatures and organics in planetary systems.

In addition to the scientific goals, PEPSci aims at establishing a long-term, cross-disciplinary network of excellent scientists in the Netherlands who are well established in the fields of earth sciences, biology, chemistry, and astronomy. Since the kick-off in 2013, several network meetings have taken place and many more researchers working on related topics have joined the network.

## References

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# The Dutch Astrochemistry Network

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**Keywords:** Astrochemistry, astronomy, chemistry, molecular physics

The Dutch Astrochemistry Network (DAN) is a highly interdisciplinary network combining the astronomical and chemical expertise in the Netherlands with the goal of understanding the origin and evolution of molecules in space and their role in the Universe. DAN was established in 2010, and funded by NWO as an integrated and coherent program of astrochemical and astrophysical experiments, quantum chemical calculations, and laboratory spectroscopy of astronomically relevant species in combination with an active program on modeling and observations of astronomical sources.

In 2016, twelve projects were selected in the second phase of the programme. DAN II focuses on three major astrochemical themes where Dutch astronomy and chemistry have particular strong expertise and experience as well as access to unique observational or experimental facilities. These three themes are 1) The Gaseous Molecular Universe where formation and destruction as well as the excitation of simple molecules are studied; 2) The Icy Universe where the role of ices is studied in the origin of molecular complexity in the Universe; 3) The Aromatic Universe, which studies the contribution of aromatic species to the molecular inventory and their evolution in space. The three themes are complementary with projects addressing common science questions from different perspectives including the photostability of small and large hydrocarbons and their reaction products, the interaction of water with grains and with PAHs, and photodissociation in the gas phase and in ice environments.

## References

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# Predicting the evolution of microbes

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**Keywords:** predicting evolution, microbial ecosystems, in silico evolution, cross-feeding

Microbes are staggeringly diverse. They can differ in almost all of their characteristics including nutritional needs and ecological function: some can synthesize all compounds required for growth themselves, while others produce only a subset, depending on metabolite exchange with partners for survival. Still others produce toxins to kill off competitors, or produce public goods to the benefit of all. Typically, microbial communities consist of many different species and are complex and highly structured. Whether the type of microbes and communities that evolves depends on chance events in its evolutionary history, or is mainly determined by environmental selection (and thus predictable) is an open question.

To answer this question we used an individual-based model to repeat the evolution of a community of digital microbes under the exact same constant conditions. To reproduce, microbes must convert a provided resource to two building block metabolites and an energy carrier, using an artificial chemistry consisting of 43 reactions and 5 intermediate metabolites. We implement many relevant organizational levels (e.g. genes, genomes, possible reactions, spatial environment), but do not explicitly model any metabolic strategies, trade-offs or ecological interactions. Instead, we let these evolve via emergent interactions, and characterize the evolved solutions.

Replicate evolutionary simulations, starting from the same population and only differing with respect to mutations, result in two types of communities: those formed by two obligately cross-feeding lineages each specialized on producing a single building block, and ecosystem composed of a single, self-sufficient lineage that synthesizes both. Which of the two communities evolves is contingent on the evolved energy metabolism. While the requirements for reproduction are identical for all microbes, the large degree of freedom allows different solutions, and the evolved solution sets limitations on future ecological roles. This suggests that mutation-level events can blow up to shape whole ecosystems via new emergent functions.

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# Emergent catalytic properties in a self-replicating system

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**Keywords:** dynamic combinatorial chemistry, autocatalysis, emergent properties, self-replication

It is very difficult to predict how a system will behave as it becomes more and more complex. A single neuron, for example, can generate action potentials, but a complex network of them can lead to something as impressive as the human brain. We have attempted to incorporate increasing complexity in our systems.

The systems that we work with are based on a small aromatic core containing two thiol groups and a small peptide tail (see Figure 1). The thiol groups can be oxidized to form disulfide bonds, introducing reversibility in the system due to disulfide exchange. Certain sizes of macrocycles can be stabilized by β-sheet- and π-π interactions, causing them to start stacking on top of one another. Fiber ends have a templating effect on the rest of the library, amplifying the macrocycle size that is most stabilized. When these libraries are mechanically agitated, the fibers can enter a growth-breakage cycle1 that increases the amount of fiber ends, causing a further, exponential amplification of the preferred macrocycle.

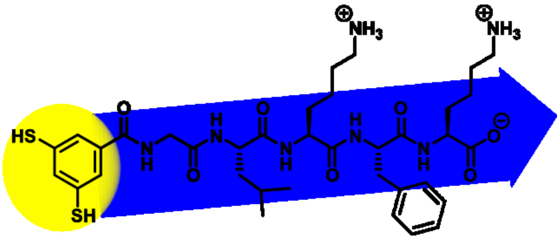

*Figure 1: A typical building block*

In this study, we have created a self-replicating system that increases in complexity as it progresses; it is capable of catalyzing another chemical reaction (the retro-aldol reaction) as the autocatalytic species grows. We have used UPLC to monitor the composition of the libraries and UV/Vis to monitor the catalytic activity towards the retro-aldol reaction.

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# Beyond vital mud and more

Jos van Oijen

As it seems quite difficult to recognize fossil remnants of supposed bacterial life in Martian meteorites, how unlikely would it be to find earthly traces of the ‘Vital Mud’ as brought forward by the late mister Alexander Graham Cairns-Smith, organic chemist in Glasgow. What however would be the chances of seeing suspected traces of higher evolved organisms that could have reached a ‘bacterial’, ‘prokaryotic’ level on the bases formulated by Cairns-Smith. His clay hypothesis is working with (much) larger ‘bio’ building blocks, so we have to deal with different standards. Then silicon offers more possibilities to review a number of other geo(morpho)logic aspects.

This poster is an invitation to consider some phenomena with an unusual look; are we dealing with pseudo(ichno)fossils or do they come from an yet unknown reality, even from a lifeless thought interior of the Earth (or other planets)?

# Self-replicating peptide nucleic acids

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**Keywords:** self-replication, nucleobases, origin of life.

The conditions that led to the formation of the first organisms and the way that life originates from a lifeless chemical soup several billion years ago are poorly understood. However, it is considered that there is a close linkage between amino acids and genetic code that may extend to the origin of life. We have previously discovered that small peptides can organize themselves into rings and subsequently form stacks, leading to self-replicating molecules-molecules that are able to make copies of themselves.[1] Cooperation between RNA and peptides may give rise to life-like behavior even with simple fully synthetic building blocks. Herein, we investigate (i) whether peptide nucleic acids can self-replicate without the need of base pair interactions and (ii) the tendency of a guanine (G) containing building blocks to self-assemble, as G is known to assemble in quadruplexes.[2] We have designed a series of nucleobase functionalized building blocks, containing a dithiol core appended to a nucleobase and terminated by an amino acid. By varying the peptide sequence and the nature of the nucleobase, a large range of peptide nucleic acid macrocycles was accessed and found to self-assemble into fibrillar nanostructures. Seeding experiments revealed the autocatalytic nature of the species formed. Interestingly, in the case of guanine, a different pattern emerged, consisting of a family of larger oligomers (up to 25mer). Upon addition of 1M of potassium bromide (KBr), only the trimer macrocycle was observed and Circular Dichroism (CD) experiments suggest the formation of G-quaduplexes.[2] We are currently investigating the molecular organization of the G-quadruplex and the effect of oligonucleotides in the amplification of specific members of the dynamic network. Nucleic acids have a unique place in contemporary life and this work might pave the way for life-like behavior with fully synthetic chemical systems.

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# Spatial regulation of synthetic cell division: the Min protein system.

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**Keywords:** Min proteins, synthetic cell.

We aim at engineering synthetic cells that autonomously will be able to perform cell division. Here we focus on studying a protein system, which functions as a spatial regulator coordinating the division machinery to mid-cell position.

MinCDE proteins are a reaction-diffusion system that spatially regulates the positioning of FtsZ–based cell-division machinery in many bacteria. Specific interactions between MinD, MinE and the membrane result in oscillation of Min proteins between the cell poles. This generates a spatiotemporal membrane gradient of MinC, allowing for FtsZ polymerization only in the mid-cell. We aim to use this protein division machinery for the synthetic cell division. Full understanding of Min system regulation is therefore crucial for its proper application.

Our studies of the Min proteins in shape-manipulated bacteria, and Min proteins reconstituted in microfabricated chambers indicate substantial differences in their dynamics and dimensions. In order to find the source of these differences we study how Min proteins behavior depends on different biochemical and physical parameters, which differ in vitro and in vivo conditions. We use microfabricated chambers covered with lipid membrane, in which we reconstitute Min proteins and observe their dynamic behavior. Using this system, we investigate the effect of cellular components as well as the effect of Min proteins concentration and volume above the membrane. Our results indicate that the Min patterns dynamics is strongly dependent on volume of protein reservoir, which is an underestimated parameter in many in vitro experiments. This may explain the discrepancy between Min behavior in vitro and in living cells.

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# Natural abiogenic methane production during fluid-rock interaction

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**Keywords:** serpentinization, abiogenic methane, catalysis.

The occurrence of abiogenic hydrocarbons, particularly methane ($CH_4$), has been recognized in a variety of geological settings on Earth and has significant implications for a range of topics, encompassing the global carbon cycle, the distribution of life within the deep subsurface and the origin of life. Several investigations also suggest the presence of abiogenic $CH_4$ on other rocky planets. Thus understanding the mechanisms of natural abiogenic hydrocarbon formation is critical. Particularly mantle peridotite hydration (serpentinization) has been invoked to play a key role in abiogenic $CH_4$ synthesis. Although $CH_4$ synthesis is known to occur in the presence of metal alloys or chromite during serpentinization at T>200 °C, little is known about the potential for $CH_4$ catalysis within or near the temperature limits of life. Here, we present results of our investigations into catalysis of low-temperature production of abiogenic $CH_4$ at largest onshore abiogenic $CH_4$ seep on Earth (Chimaera, Turkey). Carbon required for $CH_4$ synthesis is provided through limestone dissolution and a hydrogeological aquifer system that is connected to the peridotite. Hydrogen is generated through massive Fe-oxidation during peridotite alteration. The combination of bulk-rock $Fe^{3+}$ and serpentine mineral chemistry analysis with magnetization analysis implies that at Chimera oxidation ($Fe^{3+}$ content up to 85%) and $H_2$-production occurred with negligible magnetite production (0.5-1%) and incorporation of $Fe^{3+}$ into serpentine. As the serpentinites are particularly enriched in altered chromite and lack Ni-Fe alloys, we argue that $CH_4$ catalysis occurs within the mesoporous network of a nanocrystalline spinel phase, a product of chromite alteration. Nanoscale imaging shows that the spinel pore network has a strong preferred pore wall orientation and high surface area aiding catalytic reactions. We conclude that although $CH_4$ formation is kinetically hindered over carbonate precipitation, environments such as the one investigated here can sustain large fluxes of abiogenic $CH_4$ over geological timescales.

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# Building a synthetic cell: Long-term metabolic energy generation inside lipid vesicles

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Keywords: ATP generation, arginine deiminase pathway, synthetic cell.

The arginine deiminase (ADI) pathway provides a simple route for generating metabolic energy. The pathway consists of one membrane transporter and three cytosolic proteins, which produce ATP from arginine breakdown. All components of the ADI pathway have been purified and characterized in terms of reaction kinetics, stability and regulation. The pathway enzymes were also reconstituted in lipid vesicles together with the osmoregulatory glycine betaine transporter OpuA and the sensors PercevalHR and pyranine, to monitor ATP:ADP ratio and pH, respectively.

We show stable ATP production over several hours, even when the load on the system is varied. Furthermore, the production of ATP can be tightly controlled, since it only starts after addition of arginine. Finally, we show that the synthetic pathway performs way better than previously described ATP-regenerating systems (e.g. the creatine-phosphate/kinase system).

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# Generalizing species diversification models

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**Keywords:** Evolutionary biology, ecology, GLM, MCEM.

The mechanisms controlling species diversification are poorly understood. Sophisticated diversification models have been developed, but they focused on specific cases and no general method to study the combined effect of ecological factors exists.

No general method has been developed for several reasons. Firstly, evolutionary processes have extremely complex dynamics. Secondly, decay and fossilization degrade crucial evidence useful for phylogenetic analyses. Thirdly, diversification processes have many potential explanatory variables, which increases the dimensionality of the models enormously.

To overcome these issues, we propose a general diversification model expressing the evolutionary species diversification dynamics as a combination of two generalized linear models. The fact that we typically only have data on extant species can be described as a missing data problem for which we developed an MCEM-type algorithm.

We show that our method performs well for cases where an exact solution is available, and discuss potential future usage of our approach

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# High-resolution spectroscopy of gas phase aromatic molecules

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**Keywords:** Poly Aromatic Hydrocarbons, Diffuse Interstellar Bands, REMPI spectra

Polycyclic Aromatic Hydrocarbons (PAHs) are observed in interstellar space by the fluorescent radiation they emit in infrared yielding the astronomical Aromatic Infrared Bands (AIBs). Although they are ubiquitous, it is unknown what specific PAHs are present and molecular specificity is required. Employing IR-UV double resonance spectroscopy on PAHs we hope to link spectral variations in the AIBs to specific molecular structures. Moreover, we are looking for a link between PAHs and the UV/visible absorption lines observed in space, the so-called Diffuse Interstellar Bands (DIBs), by means of (1+1') REMPI spectroscopy. We will present the (1+1') REMPI spectra of increasingly larger PAHs starting with 6 rings.

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# Low temperature carbonates as indicators of early life and their implications for Mars

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**Keywords:** carbonates, Mars, isotopes, life.

Carbonates are ubiquitous in the geologic record over Earth's history and are found on Mars and within meteorites. The chemical and isotopic compositions of such carbonates have been used to constrain the composition of ancient oceans and the prevailing conditions during the development of life and its subsequent rapid evolution. The chemical composition of carbonate minerals reflects the environmental conditions under which they were formed. Recent studies have shown that microorganisms can produce carbonates with a geochemical signature that differs to those formed abiotically. The goal of our research is to develop a detailed understanding of how carbonates form and determine how the chemical composition is influenced by temperature, water composition and type of microorganisms. This will allow us to address if life had a role in the formation of the oldest carbonate deposits on Earth and potentially on Mars and other planetary systems. This study integrates field studies, state-of-the-art laboratory experiments and Sr-Mg-Fe isotope analysis to investigate the processes and environmental conditions that control the chemical and isotopic composition of low temperature (<50° C) carbonates. The role of inorganic-organic interactions will be evaluated in a natural field laboratory and in carefully controlled laboratory experiments performed under abiotic and biotic conditions. The observed geochemical and coupled stable Sr-Mg-Fe isotope variations is modelled in terms of system parameters (e.g., solution chemistry, temperature, pH, Eh) and processes (e.g., chelation, dehydration kinetics) that promote local environmental conditions that facilitate the formation of carbonate minerals in the presence of organic molecules produced by microorganisms. We hypothesise that chemical and stable isotope fractionation in biotic carbonates are controlled by enzyme mediated hydration of cations during binding to nucleation sites. Carbonates represent a robust proxy of biological activity that can be used to determine the specific environmental conditions for formation of Terrestrial and Martian carbonates

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# Building a synthetic cell: Cell volume regulation by the ABC-Transporter OpuA

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**Keywords:** ABC Transporter OpuA, volume regulation, arginine deiminase pathway, synthetic cell.

We present a synthetic vesicle system capable of regenerating ATP and response to osmotic shock. The system contains the arginine deiminase (ADI) pathway for energy production in the form of ATP. This energy is utilized by the ABC-transporter OpuA to react to osmotic stress. OpuA is activated by elevated ionic strength and imports the compatible solute glycine betaine upon hydrolysis of ATP. Differences in glycine betaine concentration form an osmotic gradient over the membrane which restores the volume through diffusion of water.

We show glycine betaine uptake over the time course of several hours. Moreover, the vesicle system allows us to switch on ATP production by the external presence of arginine. The switchable character and durable uptake make this system unique compared to alternatives as for instance ATP regeneration by creatine kinase. This allows us to study the basic mechanism of osmoprotection by OpuA and provides useful building blocks for the synthesis of a bottom-up synthetic cell.

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# Predicting the evolution of our cosmic neighborhood

Gijs Verdoes Kleijn

Abstract: Which research must be performed today to enhance the viability of humankind on timescales beyond 1e4 years? Taking stock of our cosmic environment is a fundamental ingredient in addressing this question. I will present an overview on the limits of our knowledge regarding our neigborhood out to 100 lightyears and its dynamical evolution. Current and future large astronomical surveys can help serendipitously to narrow this knowledge gap. I will illustrate this with examples on asteroids and local stellar demography with the on-going surveys Gaia and the Kilo-Degree Survey. Upcoming surveys such as Euclid in combination with E-ELT follow-up can improve significantly on this. I will outline the main scientific and technical challenges in achieving this. I conclude by showing how this astronomical topic fits into the new multi-disciplinary research field on long-term viability of humankind.

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# Epigenetic systems performance and its contribution to a diseased state: Dynamics and cell-cell variability

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**Keywords**: Epigenetic gene regulation, Synthetic systems Biology, Breast cancer

Epigenetic gene regulation is crucial for cell type specific gene expression in higher eukaryotes. We question how complex molecular interactions of epigenetic systems performance confer phenotypic stability while allowing changes to environmental cues. Computational stochastic simulation is used in combination with engineered (synthetic) mammalian cell systems and tools to modulate (trans)genes and the epigenetic state. MS2 transcript tagging and single molecule RNA FISH serve as systematic, quantitative measurements of transcription dynamics as function of the epigenetic chromatin state in single cells. We show that chromatin connectivity introduces epigenetic chromatin state switching in single genes, that mRNA statistics is gene location dependent and that the precise relationship between transcript number and cell volume sets transcriptional stochasticity and (1-3).

We focus on the role of epigenetic cell state switching in estrogen receptor positive (ER+) breast cancer endocrine therapy resistance development. ER+ breast cancer cells are strikingly heterogeneous and upon endocrine treatment defined cancer subpopulations drive resistance development (4). We study whether cell-cell variability in gene expression allows particular cell types to escape from treatment and how epigenetic plasticity affects stochastic noise in such gene regulatory networks taking transcriptional bursting into account. Our approach of modeling and quantitative sampling in engineered cells opens an unexplored field of research with great potential for medicine.

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# Shedding light on the lipid membrane of LUCA through the analysis of lipid biosynthetic pathways

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**Keywords:** Archaea, Bacteria, Lipid membrane, 'lipid divide'.

The lipid membrane is one of the most characteristic traits distinguishing the three domains of life. Membrane lipids of Bacteria and Eukarya are composed of fatty acids linked to glycerol-3-phosphate (G3P) via ester bonds, while those of Archaea have isoprene-based alkyl chains linked by ether linkages to glycerol-1-phosphate (G1P), resulting in the opposite stereochemistry of the glycerol phosphate backbone[1]. The segregation of these different lipid membranes, or so-called 'lipid divide', in the Last Universal Common Ancestor (LUCA) is a controversial topic in the evolution of microbial life since eukaryotes are thought to have evolved from Archaea, which would imply a radical change in the membrane composition[2].

In our search for the lipid biosynthetic pathways of microorganisms that can shed light on the 'lipid divide', we generated metagenomes from the anoxic water column of the Black Sea. Three bins abundant at 2000 m depth were affiliated to the FCB bacterial group *Ca*. Cloacimonadetes. These three bins had the genes coding for the enzymes involved in the formation of phospholipid fatty acids as expected for bacterial genomes. Unexpectedly, the three bacterial bins also harbored a homolog of the geranylgeranylglyceryl phosphate (GGGP) synthase, enzyme involved in the formation of the first ether bond between G1P and polyprenyl diphosphates in the archaeal membrane lipid biosynthesis, an archaeal homologue of the digeranylgeranylglyceryl phosphate (DGGGP) synthase catalyzing the second ether bond to G1P, as well as geranylgeranyl reductases to saturate the side chains. As these genome bins lack the gene to synthesize G1P, we hypothesize that they have the genetic capacity to synthesize mixed bacterial/archaeal membranes and/or G3P-based 'chimeric lipids', as recently suggested for the marine euryarchaeota group II and 'Lokiarchaeota', recently discovered descendants of the archaeal ancestor leading to eukaryotes[3]. These examples might reflect the 'archaea-to-eukaryote' membrane transition stage leading to the current 'lipid divide'.

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# Plasticity of carbon concentrating mechanisms favors earliest evolved phytoplankton in high $CO_2$ oceans

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Photosynthesis evolved in oceans of a distant past, when $CO_2$ partial pressure was high. Over time $p$CO$_2$ dropped and primary producers required carbon-concentrating mechanisms (CCMs) to supply their carbon fixing enzymes with sufficient inorganic carbon ($C_i$). At present-day $p$CO$_2$, phytoplankton groups with an earlier origin exhibit a higher CCM activity with stronger intracellular $C_i$ accumulation than their younger counterparts. We tested whether these earlier evolved groups show a stronger down-regulation of CCMs under elevated $p$CO$_2$, and found evolutionary differences in CCM plasticity. Specifically, photosynthetic $CO_2$ affinities decreased for cyanobacteria, dinoflagellates and green algae under elevated $p$CO$_2$, while maximum photosynthetic rates remained unaffected for all groups. Thus, phytoplankton groups with an earlier origin possess a higher CCM plasticity than more recently evolved groups, increasing their potential to benefit stronger from the predicted increases in $p$CO$_2$.

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