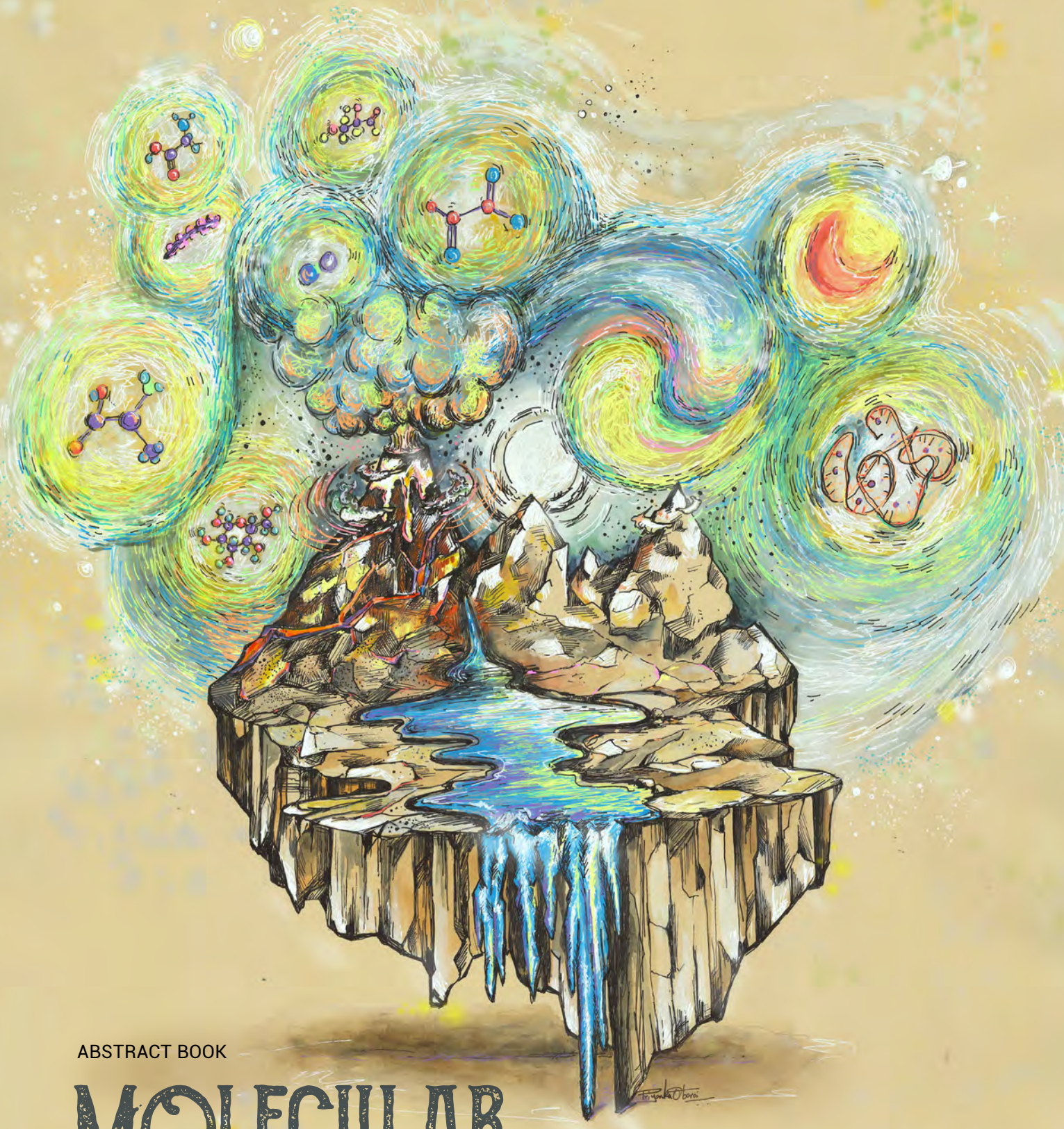
https://meetanyway.com/events/molecular-origins-of-life-munich-2020/space



ABSTRACT BOOK

MOLECULAR ORIGINS OF LIFE

CRC 235 - EMERGENCE OF LIFE CONFERENCE . ONLINE CONFERENCE . 8TH-10TH JUL 2020

IMPRINT

Scientific Organizer : Dieter Braun (LMU Munich)
Academic Organizer : Filiz Çivril (Collaborative Research Center 235 - Emergence of Life)

This event is organized by CRC 235 - Emergence of Life management and financially supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) through Project-ID 364653263 – TRR 235 and under Germany's Excellence Strategy - EXC-2094 - 390783311

CRC 235 : http://www.emergence-of-life.de/
Origins Clusters : https://www.origins-cluster.de/en/

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WELCOME ADDRESS

by Dieter Braun

Dear Emergence of Life researcher!

Evolution means to adapt to changing boundary conditions. The virtual format of the Molecular Origins of Life, Munich (MOM) conference offers many positive aspects.

This year we will be hosting many more attendees than the previous years. And the time you lose at the airports and for transfers can now be used for scientific discussions.

Besides the short talks and the interactive panel discussion format you know from previous MOMs, this time we will also have 'Meet the Speakers' sessions and what I think will be very productive; parallel poster sessions along with the talks using your browser. So besides listening to the talks over Zoom, you can look around and chat with the poster presenters.

In the evening, we will have a virtual hangout to chat and have a drink and visit more posters.

As we are learning to communicate over screens in a pleasant way, our otherwise distributed collaboration network can use this opportunity to get closer. While in the past it was difficult to hold meetings with more than 2 PIs at one location, meeting with many more across the globe is becoming very efficient.

The field of Emergence of Life has a small number of very specialized experts distributed all over the world. We should take the best out of Corona lockdown; reach out to neighboring experts, trigger collaborations and make more connections. I am optimistic that this difficult situation will have the positive effect of catalyzing the formation of 'Emergence of Life' as a scientific field similar to any other specialization.

Looking forward to meeting you!

Dieter Braun.

CODE OF CONDUCT

Inappropriate/illegal behavior and/or harassment of any kind will not be tolerated at Molecular Origins of Life, Munich virtual conference.

This includes, but not limited to,

- comments and content that are offensive or inflammatory due to gender, gender identity or expression, race, religion, ethnicity, lifestyle, age, physical appearance or disability
- inappropriate contact, sexual attention or innuendo, deliberate intimidation, stalking, and screenshots and/or recordings of individuals without consent screenshot
- and/or recordings of scientific content without consent

Participants who refuse to follow this code can face temporary/ permanent ban from the Molecular Origins of Life, Munich virtual conference and other CRC235 – Emergence of Life events.

EVENT PLATFORM MAP & GUIDE

AUDITORIUM (Floor 0)

STAGE
Zoom Webinar connection to the Conference Talks & Panel Discussions

PUZZLE & BEER OF THE DAY
Zoom Meeting connection to informal chat after all the talks, each speaker has a bottle of beer and a puzzle of the day to start the conversation

INFORMATION
Files and contact info

SUPPORT
Technical support tables for the platform

MEET THE SPEAKERS (Floor 1)
Zoom Meeting connection to chat with the speakers

NETWORKING (Floor 2)
Tables to meet the other conference participants either open networking or chats on # topics

FLOORS 3-12 (POSTER PRESENTATION ROOMS)

FLOOR 3
Presenters from time zones UTC + 04:30 to 12:00 - Visit at early hours of the event.
The presenters will probably not be available during the poster session.

FLOOR 4 - 10
Presenters from central Europe - Aligns with meeting schedule

Floor 11 & 12
Presenters from time zones UTC -04:00 to -07:00 - Visit at late hours of the event or during poster session

Shall you have problems to connect to the event space:
Email: erich@meetanyway.com
Chat: https://nextcloud.christofmast.de/call/n88vjxtn
(Password for chat: 171766)

AUDITORIUM

Stage (Zoom Webinar)

Puzzle & Beer of the day

Information area

Support

MEET THE SPEAKERS

Room 1 / Date
Speaker Names

Room 2 / Date
Speaker Names

Room 3 / Date
Speaker Names

Room 4 / Date
Speaker Names

NETWORKING

Open Networking
Just grab a seat somewhere and interact.

#astrophysical origins
Just grab a seat somewhere and interact.

 # early earth
Just grab a seat somewhere and interact.

 # RNA/DNA world
Just grab a seat somewhere and interact.

 # emergence of metabolism
Just grab a seat somewhere and interact.

 # prebiotic chemistry
Just grab a seat somewhere and interact.

 # systems chemistry
Just grab a seat somewhere and interact.

 # synthetic biology
Just grab a seat somewhere and interact.

FLOOR 3-12

Presenter Name(s)
Poster title

Presenter Name(s)
Poster title

Presenter Name(s)
Poster title

Presenter Name(s)
Poster title

Presenter Name(s)
Poster title

Presenter Name(s)
Poster title

Presenter Name(s)
Poster title

https://meetanyway.com/events/molecular-origins-of-life-munich-2020/space

EVENT PLATFORM FAQS

1. **How do I get to the MOM 2020 event platform?**
   The event is hosted at MeetAnyway Platform and here is the event space link:
   https://meetanyway.com/events/molecular-origins-of-life-munich-2020/space

2. **Which browser should I use?**
   Chrome is the best option and Firefox is 2nd. Edge and Internet Explorer are not supported.

3. **My camera and microphone do not work?**
   You need to allow your browser to access camera and microphone.

   Chrome -> Settings -> Privacy and security -> Camera or Microphone -> Turn on 'Ask before accessing on or off' and allow MeetAnyway to access when you open the event platform

   Firefox -> Options -> Privacy and security -> Camera or Microphone Setting -> Click off 'Block new requests asking to access your camera/microphone' and allow MeetAnyway to access when you open the event platform

4. **I cannot connect to the platform. What is the problem?**
   Please deactivate any Addons such as WebRTC Control, WebRTC Leak, etc.

5. **How do I get login details?**
   You must have received an email with the login details from CRC 235 Emergence of Life management (emergenceoflife@lmu.de). Contact them if you cannot locate the email.

6. **How can I change my password?**
   Please use the 'Forgot Password?' link at the Login page to reset your password!

7. **How can I change my profile at the event platform?**
   Please click on the '...' next to your name then on 'Profile Settings'. You can upload a photo, change your name and time zone.

8. **How do I get to the talks?**
   Please scroll to Auditorium Floor on the event platform and click to 'View Stage' and open the link with 'Zoom'.

9. **Can I join the event directly from Zoom?**
   We strongly suggest the attendees to use the platform for ease of access to the posters and to 'Meet the Speaker' sessions. Technically it is possible to directly connect to the Zoom sessions but we will not be providing the info.

10. **Why do I have to change room for 'Meet the Speaker' sessions?**

    The lectures will be hosted as Zoom Webinar due to high number of attendees. The Webinar add on allows only text interaction with the speakers and the panelists.

    The 'Meet the Speaker' sessions will be hosted as 'Zoom Meeting' so all the attendees can verbally and with image/video interact with the speaker.

11. **Do I have to be present at my poster room at all times?**
    We suggest you to be present at your poster room as much as possible when you are not attending the talks.

12. **Where do I upload my poster?**
    You will not upload your poster. Once you are in your chat room, click to share your screen to show your research to the others.

13. **How do I reach to the person whose poster I would like to see?**
    The platform provides a search option to find the location of the person. Once you are at the same location then you can chat with the presenter directly to schedule a visit.
    At the end of the abstract book there is contact details of all the attendees who allowed us to share information. So you can also send an email to the poster presenter to schedule a visit.

14. **Is there a possibility to meet the other attendees other than poster sessions?**
    Yes, the Networking Floor provides several tables to hang around and meet the others. We have also created some topic based tables if you would like to speak about a certain topic:
    # astrophysical origins
    # early earth
    # RNA/DNA world
    # emergence of metabolism
    # prebiotic chemistry
    # systems chemistry
    # synthetic biology

15. **Is there a logical order/grouping for poster floors?**
    We have grouped the presenters from similar time zones, floor number increases from east to west. It is more likely that you can reach the poster presenters at the lower floors earlier in the day and the higher floors later in the day. Floors 4 to 10 are presenters from central Europe so compatible with meeting schedule.

16. **How can I delete my account from the MeetAnyway Platform?**
    Please send an email to erich@meetanyway.com asking removal of your account from the platform after the event!

Technical Support Contact for MeetAnyway Event Platform
Erich Lehmann
erich@meetanyway.com
0176 209 566 86

PARTICIPATING IN TALKS (ZOOM WEBINAR)

A. Join the Webinar via URL

1. Install Zoom Desktop Client: https://zoom.us/client/latest/ZoomInstaller.exe
2. Go to the event space (Chrome): https://meetanyway.com/events/molecular-origins-of-life-munich-2020/space
3. Sign in & join the Stage on the Auditorium Floor
4. Run the file with Zoom application on your computer

B. Interacting in the Webinar

In a Zoom Webinar only host and panelists can talk. You can interact with the host, co-host and panelists by raising your hand, typing in chat or typing in Q&A.

I. Raise Your Hand:

1. Click the Raise Hand button at any time to indicate to the host and panelists that you have a question.
2. To lower your hand, click Lower Hand button.

II. Send Messages in Chat:

The feature is controlled by the host and might be limited during the event.

1. Click the Chat button to open the chat panel.
2. Type your message in the Text box at the bottom of the panel.
3. Press Enter to send you message.

III. Ask Questions in Q&A:

1. Click the Q&A button to open the window.
2. Type your question in the text field.
3.. If you want your question to be anonymous, check the Send Anonymously checkbox.
4. Click Send.

C. Leave the Webinar

1. Click the X at the upper-right corner of the window to exit the webinar or
2. Click the Leave Meeting button in the dialog box.

PARTICIPATING IN ZOOM MEETINGS

A. Join the Zoom meeting via URL

1. Install Zoom Link : https://zoom.us/client/latest/ZoomInstaller.exe
2. Join the video call of the room on MeetAnyway MOM2020 Platform
3. Run the file with Zoom application on your computer

Note: *A menu bar containing participant tools appears at the bottom of the Zoom meeting. This menu bar will appear and disappear as you roll your mouse over the area.*

B. Audio Controls

Using audio in a Zoom meeting requires you to have access to a microphone. Please be aware the host can mute and unmute you at any time. Check the icons in the menu bar and the participants panel to determine your current audio setting.

1. To unmute yourself and begin talking, click the Unmute button (microphone) in the bottom-left corner of the meeting window.
2. To mute yourself, click the Mute button (microphone). A red slash will appear over the microphone icon indicating that your audio is now off.
3. To test your computer microphone and speakers, click the up arrow to the right of the Microphone icon and select Audio settings.

Note: *You can switch to a different audio input device using the Audio Options button.*

C. Video Controls

1. Click the Start Video button in the menu bar at the bottom to begin your video.
2. Click the Stop Video button to stop sharing your video stream.
3. To choose a different webcam or adjust your video settings, click the up arrow to the right of the Video icon and select Video Settings.

Note: *When video is activated, display options are available in the upper right of the screen and in the upper right of each participant's window in both Speaker View and Gallery View.*

Note: *If you choose not to turn on your webcam in the meeting and video has been activated, your video window will contain either your name, email address, or a photo, depending on how your profile is set up.*

D. Send Messages in Chat

You can send a chat message to all participants in the meeting or privately to specific individuals.

Note: *Messages posted in chat prior to you joining the meeting are not visible to you in the chat panel.*

1. Click the Chat button to open the chat panel.
2. Type your message in the Text box at the bottom of the panel.
3. Press Enter to send you message.

Note: *You can send a private message to a single person by clicking the down arrow in the To: field and selecting the person's name from the list. The person's name will stay selected until you click the down arrow again and select Everyone.*

E. Nonverbal Feedback

Nonverbal feedback icons include a thumbs up & down, clap, away, etc. allowing you to let the host know what you are thinking without interrupting the meeting.

1. Click the Participants button in the menu bar to open the Participants panel.
2. Click the '...more' button to display the icons and click the icon.

Note: *Only a single icon is visible at any time. After clicking an icon, clicking a new icon will overwrite the first icon.*

Note: *Clap and thumbs up icons can be found also at the Reactions button in the menu bar.*

F. Share Your Screen

Both hosts and participants can share their screen in Zoom. However, participants cannot share if the host is already sharing, or if the host has disabled this feature for participants.

1. Click the Share Screen button on the menu bar.
2. Select the desktop or application you would like to share or select whiteboard to share a whiteboard Selecting Desktop will allow you to share everything on your desktop.
3. Click the Share Screen.
4. If you receive a chat message while you are screen sharing, the More button will blink. To view the chat message, click the More button and select Chat from the list.
5. Click the Annotate button to open the annotation menu. Use the draw tools (arrows, shapes) to direct participants' attention to an area of your screen or use the text tool to type notes on the screen.
6. Click the X in the upper right of the annotation menu to close the annotation menu.
7. Click the More icon to view additional options.
8. Click Stop Share in the small menu bar to stop sharing your screen.

Note: *When sharing your screen, the menu bar moves to the top of your screen and disappears until you roll your mouse over the area. Additional tools, such as Chat, Remote Control, and Audio options are located under the More button. To reposition the menu bar, click and drag it to another location on your computer.*

G. Leave the Webinar

1. Click the Leave Meeting option in the menu bar to exit the meeting or
2. Click the Leave Meeting button in the dialog box.

CONFERENCE SCHEDULE

TIME[1] 8TH JULY . WEDNESDAY

10:45-11:00	Welcome & Info Session by **Dieter Braun**
SESSION I	Chair : **Petra Schwille**
11:00-11:25	**Tetsuya Yomo** East China Normal Uni. *Construction and Evolution of a Synthetic Cell*
11:25-11:50	**Marileen Dogterom** TU Delft *Reconstituting Cytoskeletal Systems in Artificial Cells*
11:50-12:00	**Panel Discussion**
SESSION II	Chair : **William Orsi**
12:00-12:25	**Uwe Meierhenrich** Université Côte d'Azur *3D Presentation Rosetta-Philae - The Detection of Organic Molecules on the Surface of a Cometary Nucleus*
12:25-12:50	**Joachim Reitner** Georg-August-Uni. of Göttingen *Traces of Life in Very Old Rocks – What is Convincing and What Not?*
12:50-13:00	**Panel Discussion**
13:00-13:45	**Meet the Speakers[2]** of Session I & II
13:45-14:45	Lunch Break
14:45-15:00	Info Session by **Dieter Braun**
SESSION III	Chair : **Paola Caselli**
15:00-15:25	**Thomas Henning** MPI for Astronomy *Chemistry in Protoplanetary Disks*
15:25-15:50	**Ralph Pudritz** McMaster University *RNA Polymerization in Pre-Biotic Environments: Experiments with the Planet Simulator McMaster's Origins of Life Laboratory*
15:50-16:00	**Panel Discussion**
SESSION IV	Chair : **Philippe Schmitt-Kopplin**
16:00-16:25	**John Eiler** California Institute of Technology *Reconstructing Prebiotic and Biotic Chemistry Using Molecular Isotopic Structures*
16:25-16:50	**Elizabeth Bell** UC Los Angeles *The Role of Zircon in the Search for Earth's Earliest Biosphere*
16:50-17:00	**Panel Discussion**
17:00-17:45	**Meet the Speakers[2]** of Session III & IV
17:45-	**Puzzle & Beer of the Day[3] + Poster Session[4]**

TIME[1] 9TH JULY . THURSDAY

10:45-11:00	Welcome & Info Session by **Dieter Braun**
SESSION V	Chair : **Job Boekhoven**
11:00-11:25	**Jan van Esch** TU Delft *Approaching Biological Complexity: Beyond Self-Assembly*
11:25-11:50	**Stephen Mann** University of Bristol *Coacervate Dynamics and the Origin of Life*
11:50-12:00	**Panel Discussion**
SESSION VI	Chair : **Andres Jäschke**
12:00-12:25	**Longfei Wu** MRC LMB *Harnessing Chemical Energy for Activation and Joining of Prebiotic Building Blocks*
12:25-12:50	**Rafal Szabla** University of Edinburgh *Shedding UV Light on the Common Origins of RNA and DNA*
12:50-13:00	**Panel Discussion**
13:00-13:45	**Meet the Speakers[2]** of Session V & VI
13:45-14:45	Lunch Break
14:45-15:00	Info Session by **Dieter Braun**
SESSION VII	Chair : **Clemens Richert**
15:00-15:25	**Daniel Duzdevich** HHMI *The Sequence Space of Non-enzymatic RNA Copying*
15:25-15:50	**Nick Hud** Georgia Institute of Technology *A Self-Assembly Approach to Uncovering Possible Ancestors of RNA*
15:50-16:00	**Panel Discussion**
SESSION VIII	Chair : **Oliver Trapp**
16:00-16:25	**Lijun Zhou** HHMI *Assembly of a Functional Ribozyme from Short Oligomers by Enhanced Non-enzymatic Ligation*
16:25-16:50	**Donna Blackmond** Scripps Research *Asymmetric Amplification in Peptide-Catalyzed Formation of C4 Sugars from Nearly Racemic Amino Acids*
16:50-17:00	**Panel Discussion**
17:00-17:45	**Meet the Speakers[2]** of Session VII & VIII
17:45-	**Puzzle & Beer of the Day[3] + Poster Session[4]**

TIME[1] 10TH JULY . FRIDAY

10:45-11:00	Welcome & Info Session by **Dieter Braun**
SESSION IX	Chair : **Don Dingwell**
11:00-11:25	**Allen Nutman** University of Wollongong *How Long Ago was the Beginning? Looking for Life Signatures in ≥3.7 Billions-of-years-old Greenland Rocks*
11:25-11:50	**William Orsi** LMU Munich *Quantifying the Effects of Abiotic H2 Production on Carbon Metabolism in Serpentinization Systems*
11:50-12:00	**Panel Discussion**
SESSION X	Chair : **Friedrich Simmel**
12:00-12:25	**Sudha Rajamani** Indian Ins. of Sci. Edu. Res. *Prebiotic Selection Pressures Shape the Evolution of Protocells*
12:25-12:50	**Christophe Danelon** TU Delft *Roadmap to Building a Cell*
12:50-13:00	**Panel Discussion**
13:00-13:45	**Meet the Speakers[2]** of Session IX & X
13:45-14:45	Lunch Break
14:45-15:00	Info Session by **Dieter Braun**
SESSION XI	Chair : **Hannes Mutschler**
15:00-15:25	**Klara Hlouchova** Charles University in Prague *Searching for Early Proteins in Randomness*
15:25-15:50	**Roy Black** University of Washington *Prebiotic Membranes Bind Protocell Building Blocks and Catalyze Formation of Biopolymers*
15:50-16:00	**Panel Discussion**
SESSION XII	Chair : **Erwin Frey**
16:00-16:25	**Christoph Weber** MPI PKS *Selection via Phase Separation*
16:25-16:50	**Sergei Maslov** Uni. Illinois Urbana-Champaign *Onset of Natural Selection in Populations of Autocatalytic Heteropolymers*
16:50-17:00	**Panel Discussion**
17:00-17:45	**Meet the Speakers[2]** of Session XI & XII
17:45-	**Puzzle & Beer of the Day[3] + Poster Session[4]**

1 UTC+02:00, CEST, CEDT, MEST

2 Each Speaker will be hosted in a separate chat room that is moderated!

3 Each speaker will have a puzzle and a beer for each day to start the informal evening session in parallel to Poster Session!

4 Posters can be visited at any time, please contact the presenter!

SPEAKERS INDEX

SESSION I

Wednesday, 08 July, 11:00 CEST

CONSTRUCTION AND EVOLUTION OF A SYNTHETIC CELL

Tetsuya Yomo
Laboratory 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 synthetic cell 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 replicates the original genomic RNA.
After inner replication reaction of RNA, exhausting the nutrient molecules such as nucleic acids and so on, the liposomes containing the replicated RNA were subjected to the fusion with the other liposomes containing the nutrients and the division 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 experimental 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:
1Tsuji 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.

tetsuyayomo@gmail.com

SESSION I

Wednesday, 08 July, 11:25 CEST

RECONSTITUTING CYTOSKELETAL SYSTEMS IN ARTIFICIAL CELLS

Marileen Dogterom
Kavli Institute of Nanoscience at Delft University of Technology

In my group we are interested in understanding how dynamic and force-generating properties of the cytoskeleton contribute to the spatial organization of cells. I will highlight recent advances (and challenges) in our efforts to reconstitute minimal, functional cytoskeletal systems in artificial confinement. An example is the reconstitution of basic mitotic spindles in microfluidic droplets. These efforts fit in a long-term ambition to build, in collaboration with others, a minimal synthetic cell from scratch.

m.dogterom@tudelft.nl

SESSION II

Wednesday, 08 July, 12:00 CEST

3D* PRESENTATION ROSETTA-PHILAE - THE DETECTION OF ORGANIC MOLECULES ON THE SURFACE OF A COMETARY NUCLEUS

Uwe Meierhenrich
Université Côte d'Azur, Nice, France

ESA's Rosetta mission had made spectators from all over the world dream: On Wednesday, 12 November 2014, the Rosetta mission tried to pose the little robot Philae on the nucleus of comet 67P/Churyumov-Gerasimenko. The Rosetta Space Probe aimed to collect information about the composition of the comet nucleus during its spectacular approach to the sun[1]. Rosetta is the first probe to place itself in orbit around the comet and to place a lander on the surface of a cometary nucleus. The Rosetta probe carried 11 scientific instruments and a Philae lander which itself comprises 10 additional instruments. After 10 years of travel, the separation of the Philae lander from the Rosetta orbiter was carried out on November 12, 2014. The cometary sampling and composition (COSAC) instrument, a device onboard Philae, which we developed in an international partnership lead by the Max Planck Institute for Solar System Research, is a gas chromatograph using eight stationary phases coupled with a mass spectrometer time of flight type. 25 minutes after Philae's landing and bouncing on the cometary nucleus, COSAC successfully performed the first chemical analysis of cometary surface material that cannot be analyzed from the Earth. 16 organic molecules were identified in the cometary sample by using COSAC's MS-only mode[2]. After two additional bouncing events Philae finally landed on the cometary surface and operated for 60 h. During this time the COSAC instrument recorded 420 mass spectra in the enantioselective GC-MS mode. The identification of organic species in these mass spectra remains difficult because of the unexpected 'vertical' landing of Philae and the unexpected low amount of sample that was filled into the oven of COSAC's sample injector system. The first results of the analysis of the cometary nucleus surface by the COSAC instrument will be presented. These in situ cometary results will be interpreted in relation to laboratory experiments that allow for the simulation of cometary ices by condensing volatile molecules such as H_2O, NH_3, CO, CO_2, and CH_3OH in an ultra-high vacuum from the gas phase onto a cooled surface of T = 12 K. The room temperature residues of the cometary ice analogues were shown to contain amino acids[3], aldehydes[4] and ribose[5] as produced in form of simulated cometary ices in the laboratory[6]. The laboratory simulation experiments thereby confirm data on the chemical composition obtained by the Rosetta-Philae cometary probe.

References:
1 Meierhenrich: Comets and their Origin, Wiley-VCH, Weinheim 2015.
2 Goesmann, Meierhenrich et al.: Science 349, 2015, 497.
3 Munoz Caro, Meierhenrich et al.: Nature 412, 2004, 403–406.
4 De Marcellus, Meierhenrich et al.: Proc. Natl. Acad. Sci. USA 112, 2015, 965–970.
5 Meinert, Meierhenrich et al.: Science 352, 2016, 208–212.
6 Myrgorodaka, Meierhenrich et al.: Angew. Chem. Int. Ed. 54, 2015, 1402–1412

* Use of 3D glasses is recommended!.

uwe.meierhenrich@unice.fr

SESSION II

Wednesday, 08 July, 12:25 CEST

TRACES OF LIFE IN VERY OLD ROCKS - WHAT IS CONVINCING AND WHAT NOT?

Joachim Reitner[1,2], J.-P. Duda[1,2], M.Van Zuilen[3], M.Reinhardt[4], V.Thiel[1], H.Mißbach[1] & M.Hoppert[1]
[1] Georg-August-Universität Göttingen, Göttingen, Germany
[2] Göttingen Academy of Sciences and Humanities, Göttingen, Germany
[3] Institut de Physique du Globe de Paris, France
[4] Linnaeus University, Kalmar, Sweden

Life emerged >3.9 billion years (Gy) ago. However, it is very difficult to track this development in the geological rock record because most live traces have been wiped out by later metamorphic processes[1,2]. Organic carbon (Corg) preserved in late Hadean–early Archean metamorphic rocks might evidences the presence of life[1]. However, the Corg is not necessarily syngenetic with the formation of the host rock and could also be derived from abiotic sources (e.g., Fischer-Tropsch-type-synthesis, meteoric delivery)[1–4]. The discrimination of biological and abiotic contributions is challenging because the preserved Corg is recalcitrant and usually does not contain specific organic molecules. Moreover, $\delta^{13}C$ signatures of biological an abiotic Corg can interfere. Therefore, additional lines of evidence are required, including field observations, petrographic characteristics (e.g., microbial structures, mineral associations) and geochemistry (e.g., stable isotope signatures of inorganic metabolic products such as carbonates)[3,5,6]. In this talk, I will discuss potential pitfalls in the search for earliest life (e.g., 3.7 Gy old so-called "stromatolites" of Greenland)[1] and then demonstrate how we can verify and understand fingerprints of early live (e.g., in 3.5–3.4 Gy old primary fluid inclusions and microbialites)[3,5]. Our investigations help to validate putative traces of life in very old rocks and to develop a solid understanding of how life emerged on our planet.

References:
1 Reitner et al. (2020) Verlag Kurt Roessler Bornheim, 35–45 (ISBN: 978-3-935369-48-0)
2 Duda & Reitner (2016) Int. J. Astrobiol. 15, 161–163 (10.1017/S1473550416000276)
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SESSION III

Wednesday, 08 July, 15:00 CEST

CHEMISTRY IN PROTOPLANETARY DISKS

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Protoplanetary disks are circumstellar structures around young stars resembling the solar nebula at the time our planetary system formed. The disks are composed of gas – mostly molecular hydrogen – and a population of solid particles which are important in regulating the radiation level and thermal structure of these objects. Temperatures in the disks range from several thousand Kelvin close to the star to very low temperature of several Kelvin in the outer disk mid-plane. The disk surfaces are exposed to cosmic rays and stellar UV and Xray irradiation. The various regions of protoplanetary disks provide a very diverse environment for chemical processes with surface chemistry and molecular freeze-out playing an important role.
The talk will summarize the chemical properties of protoplanetary disks and will highlight what we know observationally about the molecular content of these objects. The observational basis for what we know about molecules in disks is provided by infrared spectroscopy from space and ground and (sub)millimeter molecular spectroscopy by facilities such as ALMA. The talk will also discuss potential routes to molecular complexity in disks which is connected to the formation of pre-biotic molecules.

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SESSION III

Wednesday, 08 July, 15:25 CEST

RNA POLYMERIZATION IN PRE-BIOTIC ENVIRONMENTS: EXPERIMENTS WITH THE PLANET SIMULATOR MCMASTER'S ORIGINS OF LIFE LABORATORY

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How did life originate on the Earth, and is it possible that it emerged on other Earth-like planets? It has long been posited that RNA could have been the first genetic materials in protocells[1]. Recent experimental advances have indicated that RNA polymers may grow by means of wet-dry cycles in prebiotic environments[2]. With the intent of performing experiments on RNA polymerization in a wide variety of planetary, pre-biotic conditions, we have designed a planet simulator that is now functioning in McMaster's Origins of Life Laboratory. The simulator allows excellent control and cycling of humidity, temperature, stellar 1rradiation (from IR to UV), gas composition, and pressure (one atmosphere and lower). We describe a number of experiments which act as a first "survey" of the large pre-biotic parameter space. in which various mixtures of nucleotides, salts, lipids, and irradiation conditions are explored for their ability to sustain RNA polymerization. We present our first results that suggest new insights into the role of wet/dry cycle design, salts (especially ammonium chloride) and UV irradiation- on the length of RNA polymers that may form.

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SESSION IV

Wednesday, 08 July, 16:00 CEST

RECONSTRUCTING PREBIOTIC AND BIOTIC CHEMISTRY USING MOLECULAR ISOTOPIC STRUCTURES

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Terrestrial life must have emerged from environments containing prebiotic organic compounds. However, our ability to reconstruct the first organic chemical systems that made these compounds, and to understand their transformation to the earliest life is hampered by several problems: We don't clearly recognize terrestrial organic matter in the rock record that pre-dates life; metamorphism has obscured much of the chemical complexity in our records of early life; attempts to study abiotic organic chemistry in the modern Earth are often contaminated due to the near ubiquity and fecundity of life; and as yet we have only a loose understanding of the chemistry that formed organics in our few samples of extra-terrestrial materials. For these reasons, much of our understanding of prebiotic chemistry rests on laboratory experiments that let us explore possible chemical synthesis pathways and environments and rule out implausible scenarios. Nevertheless, it remains imperative that we find ways to concretely link the chemistry that lab experiments prove is possible to the historical prebiotic chemistry that actually occurred, on the Earth and elsewhere.

Our presentation will explore the use of molecular isotopic structure — differences in isotopic content between non-equivalent atomic sites and proportions of multiply substituted isotopic forms of molecules — as a new means of distinguishing biotic from abiotic organics, of reconstructing relationships between substrates and products in organic reaction networks, and of testing hypotheses regarding the mechanisms and conditions of prebiotic chemistry. This approach has been enabled by a recent revolution in the capabilities of several technologies for analysis of isotopic structures, particularly mass spectrometric methods that are suitable for trace amounts of complex organic molecules. Also key are new theoretical studies of the chemical physics controlling intramolecular partitioning of isotopes. We will discuss these new tools and the ways in which they inform understanding of molecular formation, and we will present the newest findings of the application of this emerging field to the understanding of the synthesis of amino acids, nucleobases and other soluble organics from primitive carbonaceous meteorites. Finally, we will discuss the projected near-future application of these tools to the study of abiogenesis in terrestrial natural settings (e.g., serpentinites) and the study of ancient putative fossil biomass.

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SESSION IV

Wednesday, 08 July, 16:25 CEST

THE ROLE OF ZIRCON IN THE SEARCH FOR EARTH'S EARLIEST BIOSPHERE

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In recent decades, evidence has increasingly pointed to a Hadean (>4 billion years ago) Earth with relatively clement conditions, instead of the hellish and inhospitable environment of its namesake. Although crust older than ca. 4 billion years has not yet been identified, out-of-context crystals of zircon in later sediments have provided evidence for liquid water, a sedimentary cycle, and at least some long-lived, evolved crust within a few hundred million years of planetary formation. This suggests the possibility of planetary habitability far earlier than the oldest yet-confirmed microfossils. Carbonaceous materials from both early Archean metasediments in Greenland and from a Hadean detrital zircon from Western Australia are isotopically lighter than prevailing sources of inorganic carbon in the geologic record and may potentially preserve the signature of a Hadean-Eoarchean biosphere. The search for more such carbonaceous material is ongoing, and its rarity suggests the need for developing alternative lines of evidence for a Hadean biosphere. Available Hadean zircons are dominantly igneous in nature, and the presence of a biosphere is most evident in modern magmas through the assimilation of organic carbon-laden sediments to produce reduced, peraluminous "S-type" granites. Zircon-based proxies for magma composition use certain trace elements and the composition of mineral inclusions in zircon to determine the aluminosity and redox state of their host magmas. Several lines of evidence point to the presence of simultaneously peraluminous and reduced magmas in the Hadean. Further work on the timing of these signals in the zircon record may help to unravel the history of the terrestrial biosphere and may be a helpful companion for interpreting the carbon isotopic record. Further developing geochemical proxies in zircon will also allow us to better understand the composition of the Hadean igneous crust, which would have been the main source of inorganic nutrients to the early environment.

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APPROACHING BIOLOGICAL COMPLEXITY: BEYOND SELF-ASSEMBLY

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It remains a huge scientific challenge to understand and mimic the utilisation of chemical energy in biological systems to achieve the highly adaptable organisation and sophisticated functions like active transport, motility, selfrepair, replication, and adaptability. The development of biomimetic systems with similar energy consuming organisation and functions requires a radical departure from equilibrium self-assembly approaches, towards out-ofequilibrium systems driven by the continuous input of energy.
In our research we focus on the development of active materials driven by chemicals fuels. First, I will discuss how active materials can result from the transient self-assembly of synthetic molecules, driven by the consumption of a chemical fuel. In these materials, reaction rates and fuel levels, instead of equilibrium composition, determine properties such as lifetime, stiffness, and self- regeneration capability.[1-3] Then, I will discuss our recent steps to achieve temporal and spatial over fuel-driven self-assembly by the development of a chemical reaction network that allow for feedback control. Such systems will form the basis for self-organising systems and for design and construction of energy-consuming dynamic devices and materials.

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Keywords:
Self-Assembly, Supramolecular Chemistry, Active Materials

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COACERVATE DYNAMICS AND THE ORIGIN OF LIFE

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Many years ago Oparin proposed that liquid-liquid phase separated micro-droplets in the form of complex coacervates were a plausible model for the origin of life[1]. Although these ideas fell out of favour for many decades, the recent realization that membrane-free molecularly crowded coacervate droplets (condensates) play important and diverse functional roles in extant biology has refocused attention on phase separation as a possible mechanism underlying protobiological organization[2]. Recent studies in my laboratory have shown that coacervate micro-droplets exhibit high levels of molecular enrichment and biochemical activity including in vitro gene expression[3] and photosynthesis[4], can be transformed into membrane-coated protocells using lipid[5] or inorganic building blocks[6], and utilized as microscale agents for chemical communication and signalling in reaction-diffusion gradients[7,8]. Coacervate-based protocells are also capable of morphological reorganization in gradients of artificial morphogens[9], reversible structural transformation into lipid vesicles[10], light-induced assembly and disassembly for oligonucleotide trafficking[11], primitive phagocytosis[10] and predator-prey behaviour[12,13]. In this talk I will use the above studies to discuss the dynamical behaviour of coacervate protocell populations and speculate on the possible relevance of these properties in origin of life scenarios.

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SESSION VI

Thursday, 09 July, 12:00 CEST

HARNESSING CHEMICAL ENERGY FOR ACTIVATION AND JOINING OF PREBIOTIC BUILDING BLOCKS

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Life is an out of equilibrium system sustained by a continuous supply of energy. In extant biology, the generation of the primary energy currency, adenosine 5'-triphosphate (ATP), and its use in the synthesis of biomolecules require sophisticated enzymes. Before the emergence of such enzymes, alternative energy sources, perhaps assisted by simple catalysts, must have mediated the activation of carboxylates and phosphates for condensation reactions. I will talk about our recent results that the chemical energy inherent to isonitriles can be harnessed to activate nucleoside phosphates and carboxylic acids through catalysis by acid and 4,5-dicyanoimidazole under mild conditions in aqueous solution. Simultaneous activation of carboxylates and phosphates provides multiple pathways for the generation of reactive intermediates, including mixed carboxylic acid-phosphoric acid anhydrides, for the synthesis of peptidyl-RNAs, peptides, RNA oligomers and primordial phospholipids. Our results indicate that, prior to ATP, the activation and joining of prebiotic building blocks in aqueous solution from a common pool could have been driven by an unified chemical energy.

SESSION VI

Thursday, 09 July, 12:25 CEST

SHEDDING UV LIGHT ON THE COMMON ORIGINS OF RNA AND DNA

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The RNA World hypothesis assumes that ribonucleic acid was the first informational polymer on Earth that was responsible for storing genetic information as well as performing enzymatic activity. However, despite numerous efforts, prebiotic syntheses of RNA nucleotides either suffered from missing elements (e.g. lack of prebiotic sources of pure ribose)[1] or given chemical selectivity, were successful for only two out of four of the canonical building blocks[2,3]. However, recent results suggest that all key components of genetic alphabet could have been delivered prebiotically on Earth as a mixture of RNA pyrimidine and DNA purine nucleosides[4]. In this reaction sequence, UV light offers remarkable selectivity by destroying biologically irrelevant stereoisomers and driving the key chemical transformations. In this talk, I will demonstrate the key aspects of these photochemically driven reactions. I will also show how the oligomers of these building blocks could have protected themselves from the effects of photodamage formation in UV-rich prebiotic environments[5].

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THE SEQUENCE SPACE OF NONENZYMATIC RNA COPYING

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An important model system for studying RNA-based pre-biology is nonenzymatic template-directed primer extension, a posited component of RNA replication. Recent advances are Prompting challenging questions about how environmental contexts and heterogeneity of reaction components affect the sequence space and fidelity of nonenzymatic primer extension. Addressing these questions will require new and versatile methods that can routinely provide detailed information about how this reaction accesses template and product sequences.
I will introduce a new deep-sequencing tool for studying primer extension that uses a custom RNA construct, protocol, and analysis pipeline. I will briefly describe how the method was vetted, and its strengths and weaknesses. I will also discuss recent results that relate the established mechanism of primer extension to the patterns observed in the sequencing data, with a view to future experiments.

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A SELF-ASSEMBLY APPROACH TO UNCOVERING POSSIBLE ANCESTORS OF RNA

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The RNA World hypothesis, which posits that RNA existed before the advent of DNA and proteins, remains a popular and influential hypothesis. However, despite substantial progress in all areas of origins of life research, a robust and plausible prebiotic synthesis for RNA polymers has remained elusive. Persistent challenges with finding such a synthesis include nucleobase selection (from what was likely a complex mixture of molecules on the prebiotic Earth) and nucleotide polymerization (particularly the coupling of mononucleotides without a pre-existing template or chemical activation). These two challenges might share the same solution. We are investigating the possibility that RNA was preceded by a polymer that would have assembled more easily than RNA. This ancestral genetic polymer, or proto-RNA, may have been comprised of different nucleobases and, perhaps, a different backbone. In support of this hypothesis, experiments in our laboratory have revealed that a set of alternative nucleobases, or putative proto-nucleobases, can self-assemble in water and readily form plausible proto-nucleosides with ribose in good yields, two properties not observed with the nucleobases of extant RNA. Moreover, supramolecular assemblies formed by these putative proto-nucleobases exhibit an extraordinarily strong propensity to spontaneously adopt homochiral helical structures, even when not modified by a chiral substituent (e.g., without an attached sugar). Recent x-ray diffraction studies of these assemblies now provide structural details that we plan to use as constraints for determining which of the many proposed proto-RNA backbones would have been compatible with these proto-nucleobases.

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SESSION VIII

Thursday, 09 July, 16:00 CEST

ASSEMBLY OF A FUNCTIONAL RIBOZYME FROM SHORT OLIGOMERS BY ENHANCED NON-ENZYMATIC LIGATION

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The non-enzymatic replication of the primordial genetic material is thought to have enabled the evolution of the first ribozymes, leading to early forms of RNA-based life. However, the replication of oligonucleotides long enough to encode catalytic functions is problematic in many aspects including the low efficiency of template copying. As an alternative to template-directed polymerization of mononucleotides, the template-directed ligation of oligonucleotides could potentially help to assemble long RNAs from shorter oligonucleotides, which would be easier to replicate. However, the reported rate of non-enzymatic RNA ligation is extremely slow. Here we show that the rate of ligation can be greatly enhanced by employing a 3′-amino group at the 3′-end of each oligonucleotide, in combination with an N-alkyl imidazole organocatalyst. These modifications enable the rapid copying of long RNA templates by the multi-step ligation of tetranucleotide building blocks, as well as the assembly of long oligonucleotides using short splint oligonucleotides. We also demonstrate the formation of long oligonucleotides inside model prebiotic vesicles, suggesting a potential route to the assembly of artificial systems capable of evolution. Further, we show that a functional ligase ribozyme can be assembled in this manner. Three approaches of splint templates design enable efficient ligation and avoid the strong strand inhibition afterwards. We suggest that the genomes of primitive protocells may have consisted of relatively easily replicated oligonucleotides as short as 8 to 12 nucleotides in length.

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SESSION VIII

Thursday, 09 July, 16:25 CEST

ASYMMETRIC AMPLIFICATION IN PEPTIDE-CATALYZED FORMATION OF C4 SUGARS FROM NEARLY RACEMIC AMINO ACIDS

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Peptides formed from oligomerization of mixtures of amino acids under prebiotically plausible synthetic conditions are screened to identify catalysts for the formation of sugars from glycolaldehyde in buffered aqueous solution. Initial studies of libraries constructed using mixtures of enantiopure amino acids identified a number of peptides capable of inducing enantioenrichment in C4 sugars. Further studies demonstrated that enantioenriched erythrose could be synthesized in a one-pot sequential process starting from nearly racemic amino acids. Several selection levels are at play, combining physical phase behavior via eutectic partitioning with stochastic amplification in peptide formation and asymmetric catalysis of this simplified formose reaction.

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HOW LONG AGO WAS THE BEGINNING? LOOKING FOR LIFE SIGNATURES IN ≥3.7 BILLIONS-OF-YEARS-OLD GREENLAND ROCKS

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Because of continual plate tectonic activity, Earth's >3.6 billions-of-years-old (Ga) geological record only survives in about a millionth of the present crust. Most of this consists of metamorphosed granitic rocks, which will be devoid of life signatures. In contrast to the majority of Eoarchean (4.0-3.6 Ga) terranes, the 3.8-3.7 Ga Isua supracrustal (volcanic and sedimentary rock) belt in Greenland contains tectonic slices with maximum metamorphic temperatures below 550°C, as well as rare domains where deformation is low, resulting in the preservation of Eoarchean sedimentary structures. These domains form less than a trillionth of the present geological record. These are the only geological resource to cross-check the molecular clock modelling that places the emergence of life by the Eoarchean.

Since the 1970s, bulk graphite analysis of Isua metamorphosed sedimentary rocks reveals negative $\delta^{13}C_{VPDB}$ values, and debate surrounds whether this is a biogenic, or by the reaction $6FeCO_3 <-> 2Fe_2O_4 + 5CO_2 + C$, a metamorphic signature. To avoid possible metamorphic graphite, subsequent reduced carbon studies have sought silicate sedimentary rocks devoid of carbonate, and graphite from such sedimentary rocks yielded negative $\delta^{13}C_{VPDB}$ values (Rosing, 1999). This graphite has nanoscale morphologies consistent with pyrolyzation of structurally heterogeneous organic compounds during metamorphism. Iron isotopic signatures in Isua banded iron formations show isotope fractionations compatible with both biogenic and abiogenic processes (Dauphas et al., 2004). However, for many Isua carbonates, biogenic fractionation is the preferred interpretation (Craddock and Dauphas, 2011). In a departure from isotopic approaches, it is observed that units of Isua massive dolomite rocks ($CaMg2CO_3$) have seawater-like rare earth element + yttrium signatures, indicating a sedimentary origin. Given that low temperature dolomite forms by microbial mediation, this is proposed as simple, robust evidence for early life.

Physical rather than chemical life evidence is also sought. In the 1970s, globular structures in metamorphosed silica-rich sedimentary rocks were interpreted as relict microfossils, but subsequent investigations have reinterpreted these as younger abiogenic structures. In a unique low deformation domain discovered in the 2010s, ~3.7 Ga dolomitic rocks preserve shallow water sedimentary structures and stromatolites (bio-structures), with the latter restricted to only about $2m^2$ of outcrop.

Best-preserved ~3.7Ga stromatolites (the 2-3 cm high bumps with relicts of convex-upward internal layering) between planar sedimentary layering, found on only $2m^2$ of outcrop

Five decades of geological investigations have resulted in increasing and diverse lines of evidence for life on Earth by 3.7 Ga and probably by 3.85 Ga. Therefore, future research can leave the 'yes' or 'no' debate. Instead, via geologically-suitable samples, studies can focus on the early diversity of the ecological niches that life occupied and via an increasing array of stable isotope tools, its metabolic pathways. The oldest surviving sedimentary rocks on Earth are ~3.9 Ga, by which time life had probably emerged. Therefore, Mars, which has been geologically 'dead' for billions of years, might provide a better window on life's emergence.

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QUANTIFYING THE EFFECTS OF ABIOTIC H_2 PRODUCTION ON CARBON METABOLISM IN SERPENTINIZATION SYSTEMS

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The submarine alkaline hydrothermal vent theory for the emergence of life involves thermodynamic disequilibria across geochemical gradients of pH, temperature, redox and H_2. The theory holds that in pre-biotic alkaline hydrothermal vents, a primordial metabolism was characterized by CO_2 being reduced abiotically via H_2 produced abiotically from serpentinization: the naturally occurring reaction that occurs when water reacts with ultramafic seafloor rocks. How the abiotically produced hydrogen gas that is released by the serpentinization reaction is connected to carbon metabolism at hydrothermal settings in the deep sea is poorly understood, and has not yet been quantified. Here we report the first quantification of H_2 effects on metabolism of CO_2, acetate, and formate in a serpentinization setting at the Mid-Atlantic Ridge, where seafloor spreading exposes new ultramafic rocks to seawater releasing abundant abiotic H2. The results show a strong coupling between abiotic H_2 production, and the utilization of CO_2 and acetate, but revealed that high H_2 concentrations significantly reduce the amount of formate that can be metabolized by micro-organisms due to inhibition of the enzyme formate dehydrogenase. Reconstruction of the metabolic pathways involved reveal the role of acetate kinase and several carbon fixation pathways that are stimulated by the presence of H_2 in the serpentinization setting. These data provide the first constraints on how H_2 influences metabolism in modern serpentinization settings. Experimental approaches to produce a laboratory simulation of a prebiotic alkaline hydrothermal vent using an anoxic 'iron ocean' analog to the Hadean ocean have furthermore yielded preliminary results, whereby chimneys composed of green rust and white rust can be created under controlled anoxic conditions. Preliminary results show that the highly reactive green rust minerals bind and thereby concentrate high molecular weight DNA, which would have been a possibly important mechanism concentrating bio-molecules in similar alkaline hydrothermal settings in a pre-biotic world.

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PREBIOTIC SELECTION PRESSURES SHAPE THE EVOLUTION OF PROTOCELLS

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Protocells are primitive cellular entities that are thought to have emerged during the dawn of life on Earth. Their membranes would have been composed of mixtures of single chain amphiphiles such as fatty acids and their derivatives; moieties found in a complex prebiotic chemical landscape. The composition and the physico-chemical properties of these prebiological membranes would have been significantly affected and regulated by the physical environment that surrounded them. I will discuss what we have gleaned from studying the properties of prebiotically relevant membrane systems under pertinent selection pressures (e.g. varying pH, divalent ion concentrations etc). Our results demonstrate how environmental constraints could have shaped the landscape of early membranes. They also illustrate that hetergeneous membrane systems are more stable and robust to multiple selection pressures, thereby making them more suitable for supporting protocellular life.

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ROADMAP TO BUILDING A CELL

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The cell is the basic unit of life. Our group is engaged in the long-term effort to build a synthetic cell using a bottom-up biology approach. The core architecture of our minimal synthetic cell consists of a cell-free gene expression system (called PURE system) encapsulated inside a lipid vesicle compartment (called liposome). Using in-liposome synthesis of proteins from DNA templates, we aim to reconstitute four essential cellular modules: DNA replication, vesicle growth through phospholipid biosynthesis, liposome division and biogenesis of the transcription-translation machinery. Our latest results on these different research fronts will be presented. Finally, we will discuss a strategy to apply in vitro continuous evolution for the functional integration of these modules into a self-replicating autonomous cell.

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SEARCHING FOR EARLY PROTEINS IN RANDOMNESS

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The earliest proteins had to evolve from thoroughly random sequences. Because today's proteins are mostly highly evolved for specific functions and often rely on defined structural arrangements, it has been assumed that earliest proteins would not be able to support the early biosphere without a dominant or significant aid of other biomolecules (such as RNA and small cofactors).
To explore the potential of unnatural (unevolved) sequence space, we have performed a systematic computational and experimental exploration of random sequences. We found that the overall secondary structure and physicochemical properties of random and biological sequences are very similar. Random sequences can be both structured and disordered while the latter have lower aggregation properties and seem to better tolerated by living cells (Tretyachenko et al., Sci Rep 2017, 7.1: 15449). To better navigate protein sequence space, a new bioinformatic tool for combinatorial library design (CoLiDe) will be introduced, offering precise control over protein sequence composition, length and diversity (Tretyachenko & Voracek et al., submitted). This algorithm can be used to search for some functional phenomena that rely on specific amino acid composition and also to bias alphabets towards the amino acid composition of early biosphere. Two exemplary studies where protein composition was reduced to early amino acids will be shown in addition: (i) a ribosomal RNA-binding domain engineered from only 10 evolutionary old amino acids (lacking aromatic and positively charged residues), and (ii) a dephospho-CoA kinase mutated to lack all aromatic amino acids (Giacobelli et al. and Makarov et al., manuscripts in preparation). Our studies indicate that random (unevolved) sequences can give rise to both structured and disordered sequences. In addition, while early alphabets probably missed some of the most functional amino acids of today's proteins, our studies support that they could still serve specific molecular interactions and enzymatic activities.

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PREBIOTIC MEMBRANES BIND PROTOCELL BUILDING BLOCKS AND CATALYZE FORMATION OF BIOPOLYMERS

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How were the prebiotic building blocks of biopolymers brought together and then joined to form RNA and protein, and how did these polymers co-localize with membranes? Membranes form spontaneously from prebiotic amphiphiles such as fatty acids. We have investigated whether membranes composed of decanoic acid, a fatty acid found in meteorites, could have bound RNA and protein building blocks and catalyzed polymer formation. We find that these membranes do bind nucleobases, sugars, nucleosides and amino acids. Within each of these classes, some compounds bind better than others, helping to explain the limited diversity of cellular components. Moreover, binding the building blocks stabilizes the decanoic acid vesicles against the disruptive effects of various salts, explaining how protocells persisted on the early Earth.
To explore whether membranes promote the polymerization of building blocks, we dehydrated a solution containing decanoic acid vesicles and an amino acid-ethylester. We found that this procedure generates more dipeptide than dehydration in the absence of vesicles. Moreover, the dipeptide binds the vesicles better than the unjoined amino acid does. These results readily explain how peptides became associated with membranes. More broadly, we propose that biological evolution began with the evolution of increasingly stable fatty acid vesicles that bound and polymerized RNA and protein building blocks.

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SELECTION VIA PHASE SEPARATION

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Pre-biotic systems are complex aqueous mixtures composed of thousands of different heteropolymers which undergo chemical reactions. In such chemically-active, multi-component mixtures, enrichment and selection of a small set of components is crucial for the emergence of functional reaction cycles. However, in mixtures of a very large number of different components, each individual component is typically too diluted impeding the emergence of functionality through robust reaction cycles in pre-biotic mixtures.
Here, we propose a selection mechanism relevant for prebiotic mixtures based on cycles of phase separation combined with material exchange of the dense phase with a reservoir. We find a selective enrichment of components up to two orders of magnitude. The selection kinetics coincides with a growth of the dense phase up to the system volume leading to a final state where the selected components are condensed. For a prebiotic soup, our findings indicate that cycles of phase separation and material exchange with a reservoir, e.g. the accumulation DNA gel in rock pores periodically filled with DNA rich aqueous solution, could provide a mechanism for the selection and enrichment of specific heteropolymers sequences in a multi-component mixture at the origin of life.

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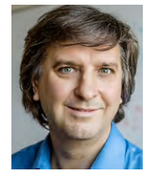
ONSET OF NATURAL SELECTION IN POPULATIONS OF AUTOCATALYTIC HETEROPOLYMERS



Sergei Maslov
Dept. of Bioengineering, Dept. of Physics, and Carl R. Woese Institute for Genomic Biology, University of Illinois at Urbana-Champaign, Urbana, IL USA

Reduction of the information entropy along with ever-increasing complexity is among the key signatures of life. Understanding the onset of such behavior in the early prebiotic world is essential for solving the problem of the origin of life. We studied a general problem of heteropolymers capable of template-assisted ligation based on Watson-Crick-like hybridization[1,2]. The system is driven out of equilibrium by cyclic changes in the environment. We modeled the dynamics of 2-mers, i.e., sequential pairs of specific monomers within the heteropolymer population[1]. While the possible number of them is Z^2 (where Z is the number of monomer types), we observe that most of the 2-mers get extinct, leaving no more than 2Z survivors. This leads to a dramatic reduction of the information entropy in the sequence space. This natural-selection-like process ultimately results in a limited subset of polymer sequences. Importantly, the set of surviving sequences depends on the initial concentrations of monomers and remains exponentially large (2^L reduced down from Z^L for chains of length L) in each of realizations. Thus, an inhomogeneity in the initial conditions allows for a massively parallel search of the sequence space for biologically functional polymers, such as ribozymes. The problem has a surprising connection[3] to microbial ecology in which multiple species (analogous to autocatalytic 2-mers) compete for essential nutrients of two types (Z types of left and right ends of chains). Finally, I describe preliminary experimental results[4] validating the predictions of our model.

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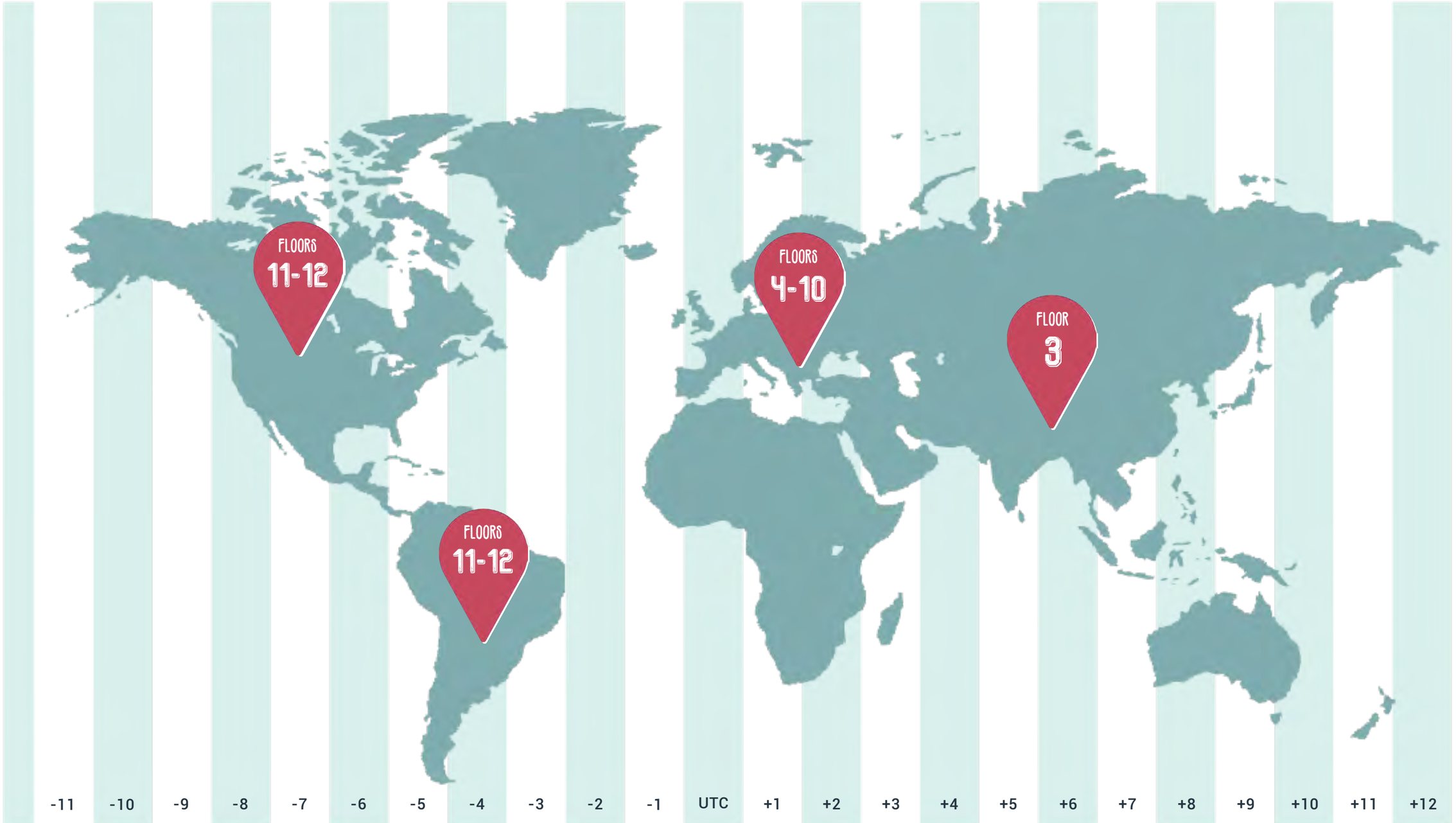

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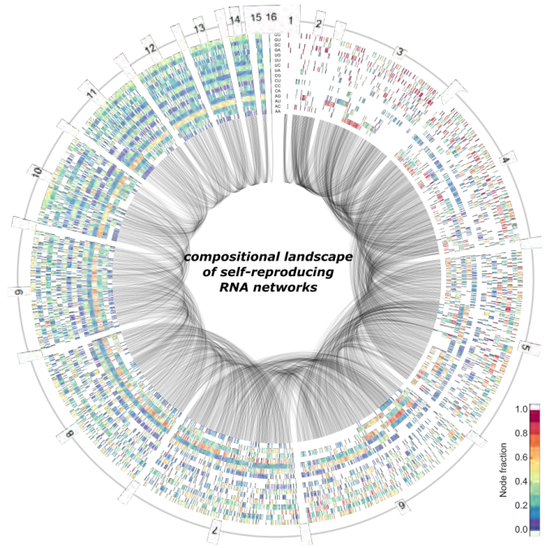

DARWINIAN PROPERTIES AND THEIR TRADE-OFFS IN AUTOCATALYTIC REACTION NETWORKS

Ameta S.[¥,1,3], Arsène S.[¥,1*], Foulon S.[1], Saudemont B.[1], Clifton B.E.[2], Griffiths A.D.[1*], Nghe P.[1*]

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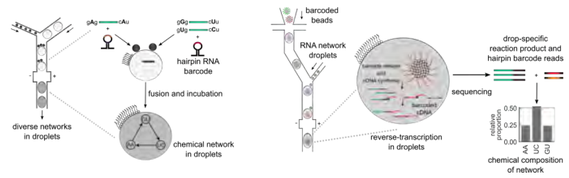
Discovering autocatalytic chemistries that can evolve is a major goal in systems chemistry and a critical step towards understanding the origin of life. Autocatalytic networks have been discovered in various chemistries[1-4], but we lack a general understanding of how network topology controls the Darwinian properties of variation, differential reproduction, and heredity, which are mediated by the chemical composition. Using barcoded sequencing and droplet microfluidics, we establish a landscape of thousands of networks of RNAs[5] (figure) that catalyze their own formation from fragments[6,7], and derive relationships between network topology and chemical composition[5]. We find that strong variations arise from catalytic innovations perturbing weakly connected networks, and that reproduction increases with global connectivity. These rules imply trade-offs between reproduction and variation, and between compositional persistence and variation along trajectories of network complexification. Overall, connectivity in reaction networks provides a lever to balance variation (to explore chemical states) with reproduction and heredity (persistence being necessary for selection to act), as required for chemical evolution.



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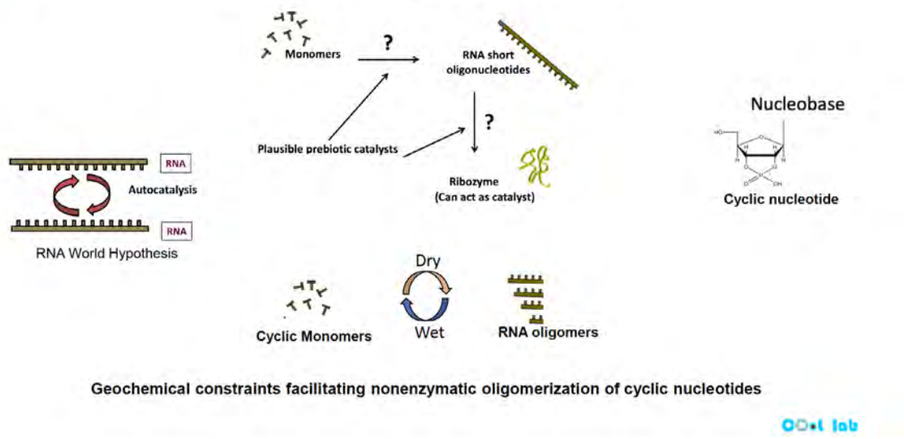

Geochemical constraints facilitating nonenzymatic oligomerization of cyclic nucleotides

GEOCHEMICAL CONSTRAINTS SHAPING THE NONENZYMATIC OLIGOMERIZATION OF CYCLIC NUCLEOTIDES

Shikha Dagar, **Susovan Sarkar and Sudha Rajamani**
Department of Biology, Indian Institute of Science Education and Research, Pune 411008, India

About one-third of the extant enzymes are metalloenzymes. This ubiquitous nature of metal ions in extant life highlights their potential role in the emergence and evolution of early life on Earth. Specifically, metal ions are thought to have played the role of catalysts on early Earth in prebiotically pertinent processes. Among several competing theories that hypothesize how life would have originated on Earth, RNA World Hypothesis happens to be the most prevalent one. It suggests that RNA would have been the first relevant biomolecule to set the stage for life's emergence, and whose formation would have been driven by nonenzymatic processes[1]. This is due to its capability to act as a catalyst in addition to being a genetic material (Carl Woese, Francis Crick and Leslie Orgel, 1960s)[2]. However, spontaneous generation of RNA, which involves energitically uphill condensation reactions among nucleotides, is thought to be non-trivial. Nonetheless, even if long RNAs could indeed form by nonenzymatic means, they would require metal ions to fold appropriately and catalyze reactions[3].

In this study, the effect of metal ions on the nonenzymatic oligomerization of prebiotically relevant cyclic nucleotides was investigated. Reactions were performed under, both, laboratory simulated prebiotic conditions, and using water samples collected from an astrobiologically relevant early Earth analogue site in Ladakh, India[4]. This was done to evaluate the robustness of the results obtained from a predetermined laboratory set up. Furthermore, it also enables an understanding of how a more 'realistic' scenario, wherein multiple entities like metal ions and other co-solutes are present, could affect the otherwise 'controlled' reactions. Under aqueous conditions, intact oligomers up to tetramers were observed. However, in the reactions performed under analogue conditions, even-though the hot-spring water samples seemed to enhance the rate of oligomerization, they also led to the quick destabilization of the resultant oligomers. Our results suggest that the presence of ions could effectively act as a selection pressure under prebiotic scenarios, thereby playing a vital role in shaping the evolutionary landscape of a putative RNA World.

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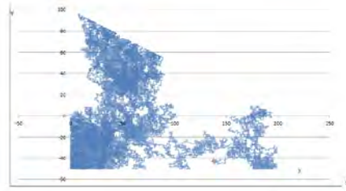
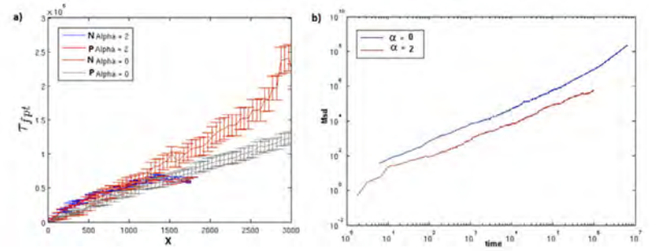
$$J = \frac{N_R - N_L}{N_R + N_L} \qquad (1)$$



current of levy walk in the ratchet



LEVY SWIMMER IN AN ASYMMETRIC CHANNEL

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We numerically study the dynamics of a model Levy walker, moving in a 2-dimensional medium confined by the walls of an asymmetric channel. We show that, as a result of both asymmetric potential due to the channel and also the power law step size distribution, the Levy walker will achieve a net directed velocity in the direction preferred by the channel. Other statistical properties of the walker such as mean first passage time and the mean square displacements are also examined.

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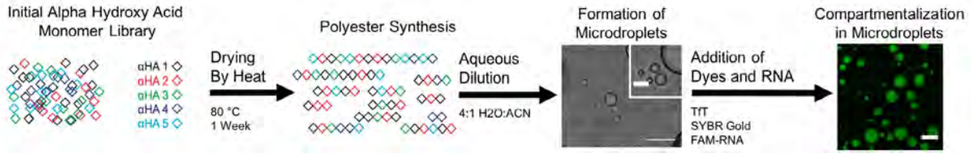

DNA LIQUID CRYSTAL COACERVATES AND POLYESTER MICRODROPLETS AS MODEL SYSTEMS IN ORIGINS OF LIFE RESEARCH

Tony Z. Jia[1,2], **Kuhan Chandru[3,4], Yayoi Hongo[1], Rehana Afrin[1], Tomohiro Usui[1,5], Kunihiro Myojo[6], H. James Cleaves II[1,2,7], Tommaso P. Fraccia[8]**

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[2] Blue Marble Space Institute of Science
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[4] Space Science Centre (ANGKASA), Institute of Climate Change, National University of Malaysia
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[6] Department of Earth and Planetary Science, Tokyo Institute of Technology
[7] Institute for Advanced Study, Princeton University
[8] Institut Pierre-Gilles de Gennes, Chimie Biologie et Innovation, ESPCI Paris, PSL University

Liquid-liquid phase separation (LLPS) controls important biological processes including catalysis and gene regulation. Due to their ease of in vitro assembly into membraneless compartments and their presence within modern cells, LLPS systems have been postulated to be one potential form that the first cells on Earth took on. Here, we present work regarding the structure, assembly, and function of various in vitro LLPS systems, such as DNA liquid crystal coacervates and polyester microdroplets, that produce membraneless compartments which may have been relevant to the emergence of primitive compartments. These compartments exhibit various properties, such as compartmentalization and self-assembly, and catalysis, potentially providing scaffolds that could have effected the assembly of more complex chemical structures. While there are still a number of remaining open questions regarding LLPS systems as models for primitive membraneless cells, including how modern biologies acquired such membraneless organelles, understanding the exact connection between LLPS systems and primitive cells will shed light into how primitive cells transitioned to modern cells.

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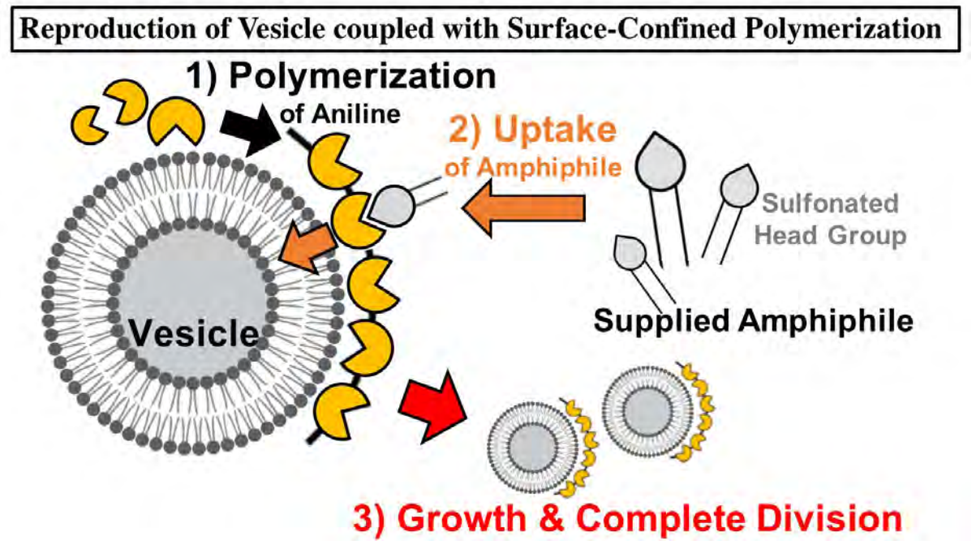

REPRODUCTION OF VESICLES COUPLED WITH A MEMBRANE SURFACE-CONFINED TEMPLATE POLYMERIZATION

Minoru Kurisu[1], **Harutaka Aoki[1], Takehiro Jimbo[1], Yuka Sakuma[1], Sandra Luginbuhl[2], Peter Walde[2], Masayuki Imai[1]**

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[2] Department of Materials, ETH Zürich, Switzerland

Molecular assembly system that have autonomous reproduction ability can be considered as minimal cell-like systems, which bridges non-living and living forms of matter[1]. Here we show the reproduction of cell-sized vesicles coupled with polymerization on the surface of vesicles. The particular reaction used is the template polymerization of aniline occurring on the surface of AOT vesicles, which yields polyaniline emeraldine salt form (PANI)[2]. When AOT micelles are microinjected to AOT vesicles during polymerization, the AOT – PANI-ES vesicles selectively incorporate them in their membrane, which leads to a growth of the vesicle. If the AOT vesicles contained cholesterol, the vesicle not only showed growth, but also division, i.e., reproduction of vesicles[3].

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GEO-ELECTROCHEMICAL DECOMPOSITION OF AMINO ACIDS ON ICY PLANETESIMALS REPRODUCES ORGANICS IN CARBONACEOUS METEORITES

Li Yamei[1], Norio Kitadai[1,2], Ryuhei Nakamura[1], Yasuhito Sekine[1]
[1] Earth-Life Science Institute, Tokyo Institute of Technology
[2] Japan Agency for Marine-Earth Science and Technology

Organics in carbonaceous meteorites are the remnants of primitive solar system chemistry and parent-body processes. Amino acids are ubiquitously found in carbonaceous chondrites, and their genesis and conversion have important implications on the origin of biomolecules, the geophysical evolution and the geochemical processes that occurred in their parent bodies (icy planetesimals).

In Murchison meteorite and several reported carbonaceous meteorites, in addition to amino acids, other types of water-soluble, low molecular weight compounds make a complex suite that includes hydroxycarboxylic acid, aliphatic monoamines, monocarboxylic acids, alcohols, and others. However, the synthetic origin for their formation leading to their occurrence in meteorites remain poorly understood, becoming a long-standing enigma.

It has been largely considered that water-rock interactions cause the alteration of organic distribution and associated minerals in carbonaceous bodies, however, how does energy transduction proceed in such environment and how the chemical processes have shaped the organic distributions remain poorly understood. Here we report that geo-electrochemical processes can decompose aliphatic amino acids into monocarboxylic acids, alcohols, amines, and hydroxycarboxylic acids. Iron and nickel sulfides work as effective catalysts for the redox-mediated activation of amino acids. Such geo-electrochemical processes are driven spontaneously by the water-rock interactions, which generate steep redox, pH and chemical gradients between the interior and exterior of the icy planetesimals.

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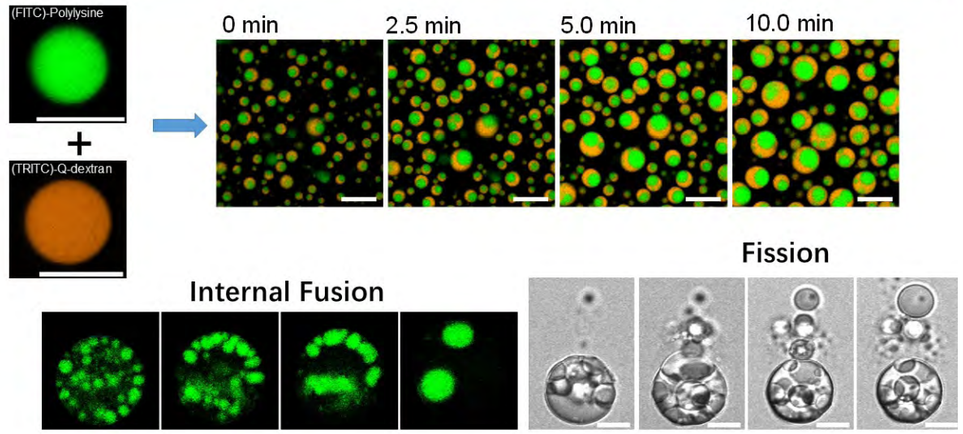

PROTOCELL WITH MEMBRANELESS "ORGANELLES" FORMED BY LIQUID-LIQUID PHASE SEPARATION

Hairong Jing, Qingwen Bai, Ya'nan Lin, Haojing Chang, Dehai Liang
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Construction of protocell with hierarchical structure and living functions by prebiotically plausible components and mechanism is still a great challenge. Growing evidences demonstrate that the membraneless organelles, which facilitate many essential cellular process, are formed by RNA, protein and other biopolymers via liquid-liquid phase separation (LLPS). The formation of protocell on the early Earth could follow the same principle. In this work, we develop a novel coacervate-based protocell containing membraneless subcompartments via spontaneous liquid-liquid phase separation simply by mixing single-stranded oligonucleotides (ss-oligo), quaternized dextran (Q-dextran), and poly(L-lysine) (PLL) together. The resulting biphasic droplet, with PLL/ss-oligo phase being the interior subcompartments and Q-dextran/ss-oligo phase as the surrounding medium, is capable of sequestering and partitioning biomolecules into distinct regions. When the droplet is exposed to salt or dextranase, the surrounding Q-dextran/ss-oligo phase experiences a dynamic adjustment and dissociates, which induce the internal subcompartments to chaotically move and fuse. Besides, the external electric field at lower strength can drive the biphasic droplet to undergo a deviated circulation concomitant with the fusion of localized subcompartments, while high-strength electric field can induce the directional movement of subcompartments and polarize the whole droplet, resulting in the release of daughter droplets in a controllable manner. Our study highlights that liquid-liquid phase separation of biopolymers is a powerful strategy to construct hierarchically structured protocells resembling the morphology and functions of living cells, and provides a step towards a better understanding of the transition mechanism from non-living to living matter under prebiotic conditions.

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Figure 1 : Schematic presentation of the template assisted peptide replication.

EMERGENCE OF NATIVE PEPTIDE SEQUENCES IN THE CONTEXT OF ORIGINS OF LIFE

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[2] Department of Chemistry, Indian Institute of Engineering Science and Technology, Shibpur, Howrah, India

Biopolymer syntheses in living cells are perfected by an elaborate error correction machinery, which was not applicable during polymerization on early Earth. Scientists are consequently striving to identify mechanisms by which functional polymers were selected and further amplified from complex prebiotic mixtures. Here we show the instrumental role of non-enzymatic replication in the enrichment of certain product(s). To this end, we analyzed a complex web of reactions in β-sheet peptide networks, focusing on the formation of specific intermediate compounds and template-assisted replication[1,2]. Remarkably, we find that the formation of several products in a mixture is not critically harmful, since efficient and selective template-assisted reactions serve as a backbone correction mechanism, namely, for keeping the concentration of the peptide containing the native backbone equal to, or even higher than, the concentrations of the other products. We suggest that these findings may shed light on molecular evolution processes that led to current biology[3].

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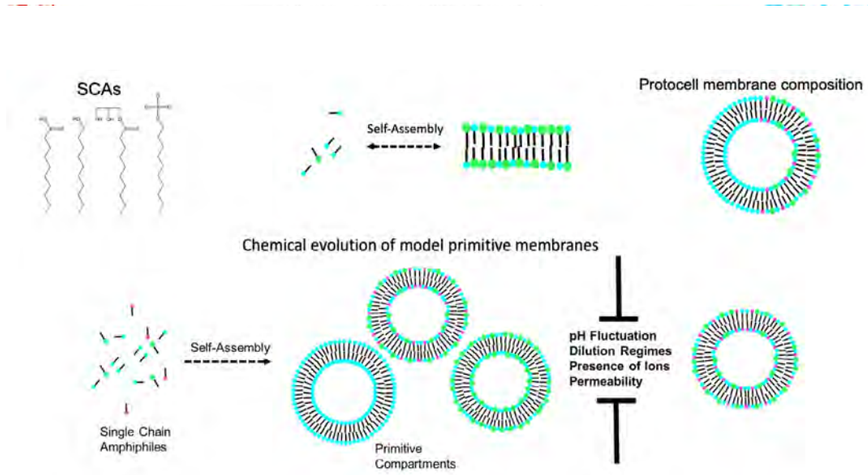

THE INFLUENCE OF COMPOSITIONAL HETEROGENEITY OF MODEL PROTOCELLULAR MEMBRANES: IMPLICATIONS FOR THE EMERGENCE OF CELLULAR LIFE

Susovan Sarkar, **Shikha Dagar, Ajay Verma, Sudha Rajamani**
Department of Biology, Indian Institute of Science Education and Research, Pune 411008, India

Protocell membranes are thought to be comprised of mixtures of single chain amphiphiles, such as fatty acids long-chain alcohols, etc. which would have been part of the complex prebiotic chemical space. The physico-chemical properties of these prebiological membranes would have been significantly affected, and regulated, by the physical environment that they were present in. In this study, the physico-chemical properties of two different chain length membrane systems i.e. C18 and C11, were systematically characterized, under prebiotically pertinent environmental conditions. The membrane systems have been designed to be composed of fatty acid and/or their corresponding alcohol and their glycerol monoester derivatives, to make a range of membrane combinations (e.g. binary and tertiary systems). The properties of those membranes were evaluated as a function of multiple factors including their composition, stability under alkaline pH, in the presence of Mg^{2+} ions, dilution regimes. The permeability of C11 based mixed membrane systems were also investigated. These environmental constraints would have acted as important prebiotic selection pressures to shape the evolution of prebiological membranes. Our results demonstrate that complex membrane systems are more stable and robust to multiple selection pressures, thereby making them more suitable for supporting protocellular life. Furthermore, different fatty acid derivatives conferred varying degrees of stability when mixed with their respective fatty acid moiety. Importantly, the aforesaid depended on the chain length of the system, and the selection pressure that was applied. Significantly, when the systems were subjected to multiple selection pressures in a consecutive manner, only the heterogeneous membrane systems survived the race. These results highlight the requirement of compositional complexity, and underscore its implications for the emergence of mixed membrane systems during the dawn of life on Earth.

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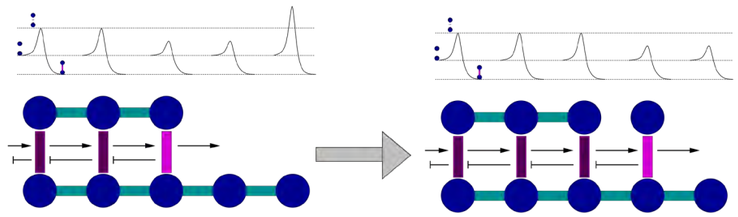
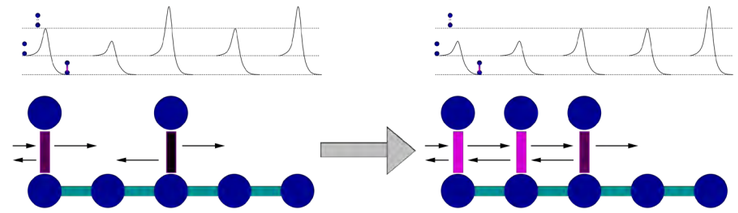


(a) Strand with asymmetric cooperativity (Evolutionarily superior)



(b) Strand with symmetric cooperativity (Evolutionarily inferior)

IDENTIFICATION OF EVOLUTIONARY ADVANTAGE OF SOME FUNDAMENTAL PROPERTIES OF DNA FROM REPLICATIVE POTENTIAL MAXIMI-ZATION OF PRIMORDIAL AUTOCATALYTIC HETEROPOLYMERS

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[2] Integrated Mathematical Oncology, H. Lee Moffitt Cancer Center and Research Institute, Tampa, FL, U.S.A

DNA in all living systems shares common properties that are remarkably well suited to its function, suggesting refinement by evolution. However, DNA also shares some counter-intuitive properties that confer no obvious benefit, such as strand directionality and anti-parallel strand orientation, which together result in the complicated lagging strand replication. The evolutionary dynamics that led to these properties of DNA remain unknown. By carefully examining the physico-chemical requirements for evolutionarily successful primordial self-replicators, we theoretically show that asymmetric uni-directional self-replicators would have an evolutionary advantage over bidirectional self-replicators. The competing requirements of low and high kinetic barriers for induction and retention of monomers respectively are simultaneously satisfied through asymmetric kinetic influence of inter-strand bonds, resulting in evolutionarily successful unidirectional self-replicators. The advantage of anti-parallel strand orientation stems from the increased rate of replication, achieved by dividing the DNA into predictable, independently and simultaneously replicating segments, as opposed to sequentially replicating the entire DNA, thereby parallelizing the replication process.

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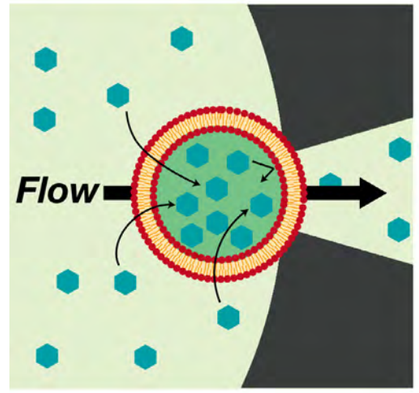

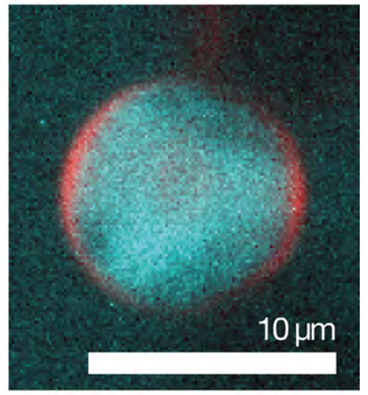

ABIOTIC ACCUMULATION OF SMALL MOLECULES AND IONS INTO CELLULAR COMPARTMENT AGAINST A CONCENTRATION GRADIENT

Hironori Sugiyama[1], **Toshihisa Osaki[2,3], Shoji Takeuchi[2,4], Taro Toyota[1,5]**
[1] Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo
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[4] Department of Mechano-Informatics, Graduate School of Information Science and Technology, The University of Tokyo
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At the emergence of cell-like chemical systems at the origin of life, compartment is one of indispensable elements[1]. On one hand, com-partmentalization is advantageous for the stable self-replication cycle against the parasitic molecules[2,3]. On the other hand, low permeabil-ity of phospholipid membrane hinders repeatable and continuous supply of molecules and ions inside. An abiotic process to accumu-late substances into preformed liposomes against the concentration gradient would be prerequisite for maintenance, propagation, and development of metabolic system. In this study, we present that without proteins, cell-sized liposomes under hydrodynamic envi-ronment repeatedly accumulate small molecules and ions even against the concentration gradient. Notably, an analogue of adeno-sine triphosphate was also accumulated. We investigated this intri-guing and unexplored class of transportation of substrates across the lipid membrane with in-house-developed automated observation platform based on the microfluidic device (termed as MANSIONs). We discuss that the mechanism of this accumulation is probably ex-plained by a unique partitioning at the liposomal membrane exposed to the external flow in a constrained space. The hydrodynamic ac-cumulation could provide a breakthrough step for driving a metabo-lic pathway at the origins of life.

1 Segré et. al., The lipid world. Origins of life and evolution of the biosphere 2001, 31 (1-2), 119-145,
2 Ichihashi et.al., Darwinian evolution in a translation-coupled RNA replication system within a cell-like compartment. Nat. Commun. 2013, 4, 2494,
3 Matsumura et. al., Transient compartmentalization of RNA replicators prevents extinction due to parasites. Science 2016, 354 (6317), 1293-1296

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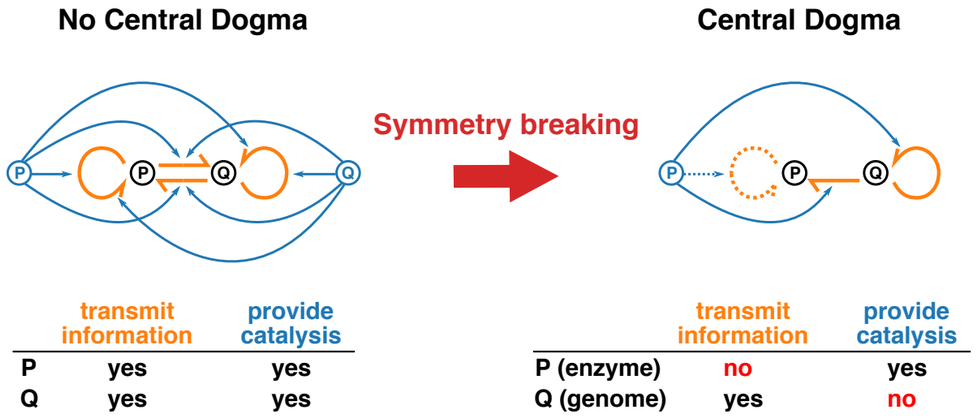

	transmit information	provide catalysis
P	yes	yes
Q	yes	yes

	transmit information	provide catalysis
P (enzyme)	no	yes
Q (genome)	yes	no

THE ORIGIN OF THE CENTRAL DOGMA THROUGH CONFLICTING MULTILEVEL SELECTION

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The central dogma of molecular biology rests on two kinds of asymmetry between genomes and enzymes: informatic asymmetry, where information flows from genomes to enzymes but not from enzymes to genomes; and catalytic asymmetry, where enzymes provide chemical catalysis but genomes do not. How did these asymmetries originate? Here we show that these asymmetries can spontaneously arise from conflict between selection at the molecular level and selection at the cellular level[1]. We developed a model consisting of a population of protocells, each containing a population of replicating catalytic molecules. The molecules are assumed to face a trade-off between serving as catalysts and serving as templates. This trade-off causes conflicting multilevel selection: serving as catalysts is favoured by selection between protocells, whereas serving as templates is favoured by selection between molecules within protocells. This conflict induces informatic and catalytic symmetry breaking, whereby the molecules differentiate into genomes and enzymes, establishing the central dogma. We show mathematically that the symmetry breaking is caused by a positive feedback between Fisher's reproductive values and the relative impact of selection at different levels. This feedback induces a division of labour between genomes and enzymes, provided variation at the molecular level is sufficiently large relative to variation at the cellular level, a condition that is expected to hinder the evolution of altruism. Taken together, our results suggest that the central dogma is a logical consequence of conflicting multilevel selection.

1 Takeuchi and Kaneko 2019 The origin of the central dogma through conflicting multilevel selection. Proc. R. Soc. B. 286 20191359 link

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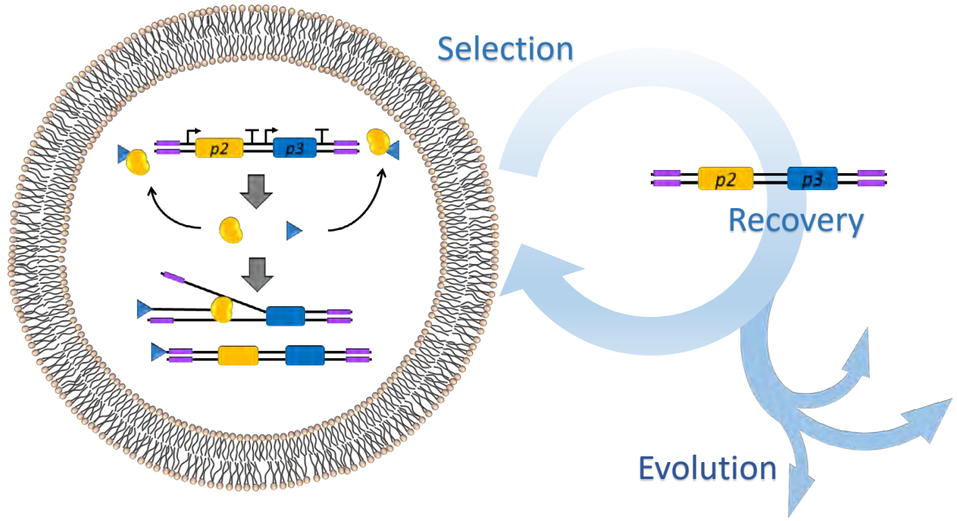

ENGINEERING EVOLVABILITY OF SELF-REPLICATING DNA AS A TOOL TOWARDS BUILDING A SYNTHETIC CELL

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A consensus is that chemical evolution preceded biological evolution, and was the main driver behind the emergence of life. Our vision is to build a synthetic cell model via evolution so that we better understand life's properties and how life originated via chemical evolution. Our goal is not to determine the most plausible evolutionary path for emergence of terrain life, but to understand broader evolutionary principles and processes that can lead to emergence of self-replicating, autonomous, functionally integrated entities. To achieve this vision, we are developing a platform for a system's level continuous in vitro evolution of a synthetic cell model. We will start by evolving a simple system composed of self-replicating DNA encoding for a viral DNA polymerase and its complementary terminal protein in liposomes. Herein, we present the work done to enable long-term directed evolution of this bi-cistronic DNA fragment. As a proof of concept, we demonstrated that single molecules of DNA can be encapsulated in a polydisperse population of giant unilamellar vesicles, and that in vitro expressed replication proteins can amplify the parental linear DNA. We also show that enrichment of self-replicating DNA can be observed from a mixture with non-self-amplifying DNA, which suggests that in-liposome evolution of a DNA polymerase is possible. Moreover, we show that engineered exonuclease-deficient DNA polymerase variants are functionally active and may be potentially used as mutator DNA polymerases in a continuous in vitro evolution scenario. This work constitutes a major milestone towards in vitro evolution of a self-replicating DNA genome in a synthetic cell model.

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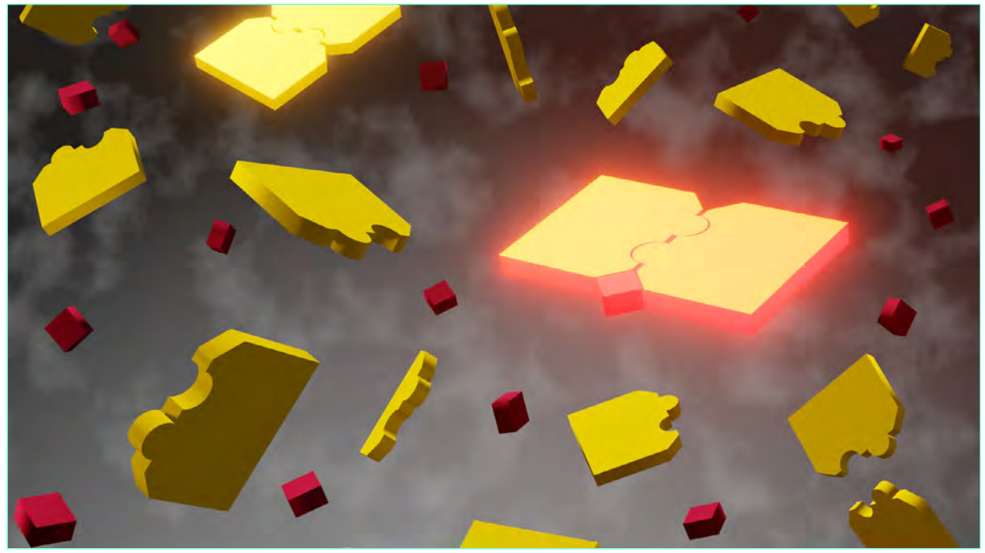

COOPERATIVELY ENHANCED REACTIVITY AND 'STABILITAXIS' OF DISSOCIATING OLIGOMERIC PROTEINS

J. Agudo-Canalejo[1], **P. Illien[2], and R. Golestanian[1,3]**
[1] Max Planck Institute for Dynamics and Self-Organization (MPIDS), D-37077 Göttingen, Germany
[2] Sorbonne Université, CNRS, Laboratoire PHENIX, UMR CNRS 8234, 75005 Paris, France
[3] Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, UK

Many functional units in biology, such as enzymes or molecular motors, are composed of several subunits that can reversibly assemble and disassemble. This includes oligomeric proteins composed of several smaller monomers, as well as protein complexes assembled from a few proteins. By studying the generic spatial transport properties of such proteins, we investigate here whether their ability to reversibly associate and dissociate may confer them a functional advantage with respect to non-dissociating proteins. In uniform environments with position-independent association-dissociation, we find that enhanced diffusion in the monomeric state coupled to reassociation into the functional oligomeric form leads to enhanced reactivity with distant targets. In non-uniform environments with position-dependent association-dissociation, caused e.g. by spatial gradients of an inhibiting chemical, we find that dissociating proteins generically tend to accumulate in regions where they are most stable, a process that we term 'stabilitaxis'.

J. Agudo-Canalejo, P. Illien, and R. Golestanian, Proc. Natl. Acad. Sci. U.S.A. (2020, in press). arXiv:1911.02350

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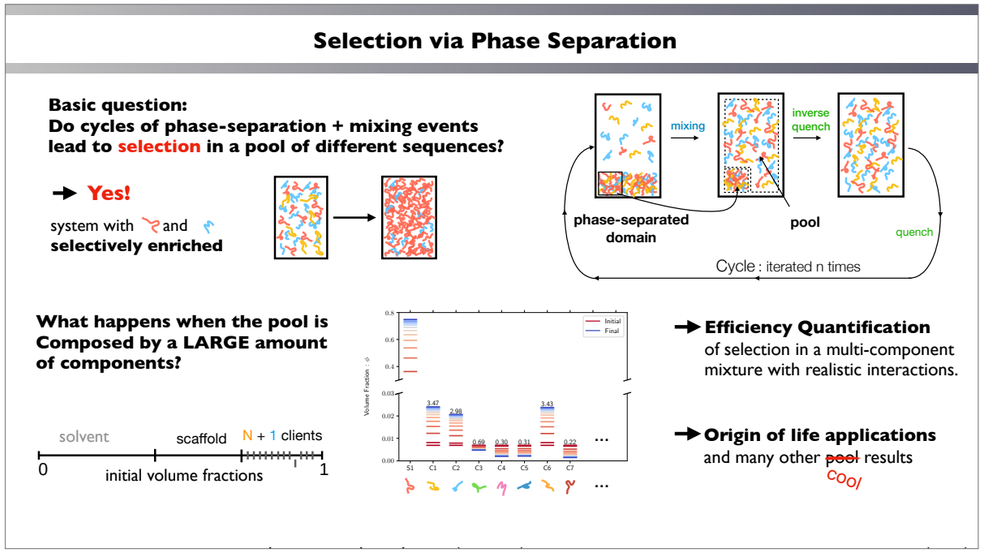

SELECTION VIA PHASE SEPARATION

Giacomo Bartolucci[1,2], **Yash Rana[1,2], Alexandra Kühnlein[3], Christof Mast[3], Dieter Braun[3], and Christoph A. Weber[1,2]**

[1]Max Planck for the Physics of Complex Systems, Dresden,
[2]Center for Systems Biology, Dresden
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Living cells and pre-biotic systems are complex aqueous mixtures composed of thousands of different heteropolymers. In such multi-component mixtures, enrichment and selection of a small set of components is important to achieve biological function. However, when the number of components increases, components are more diluted impeding a significant enrichment of selected components.

Here, we propose a selection mechanism relevant for prebiotic mixtures based on cycles of phase separation combined with material exchange of the dense phase with a reservoir. We find a selective enrichment of components up to two orders of magnitude coinciding with a growth of the dense phase up to the system volume. Such enrichment of selective components is robust also in mixtures composed of a large number of components. For a prebiotic soup, our findings indicate that cycles of phase separation and material exchange with a reservoir, e.g. the accumulation DNA gel in rock pores periodically filled with DNA rich aqueous solution[1], could provide a mechanism for the selection and enrichment of specific heteropolymers sequences in a multi-component mixture at the origin of life.

1 M. Morasch, A. Kühnlein, Christof Mast, Dieter Braun et al. Nature Chemistry 2019

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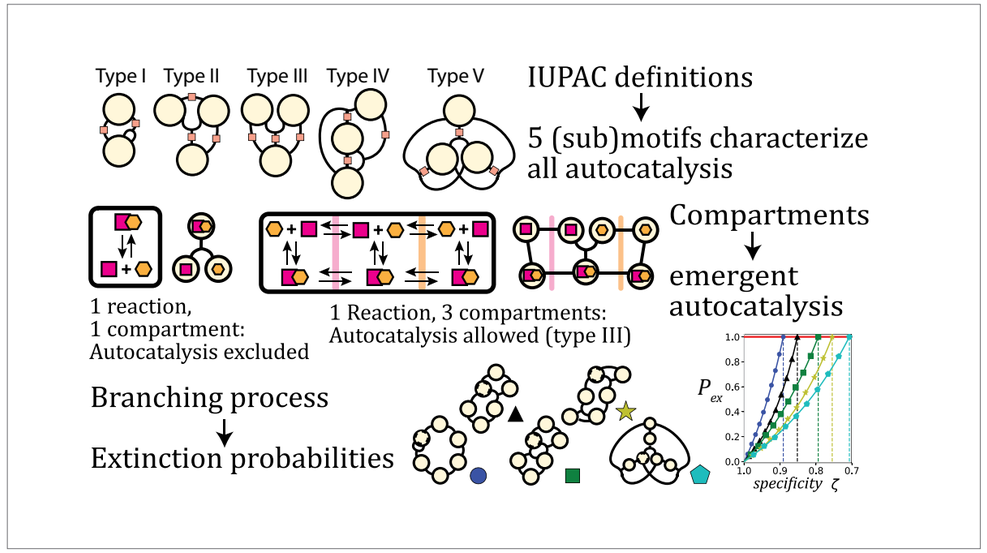

AUTOCATALYSIS IN CHEMICAL NETWORKS: UNIFICATIONS AND EXTENSIONS

Alex Blokhuis[1,2,3,4], **David Lacoste[1], Philippe Nghe[2]**

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Autocatalysis is a multifarious phenomenon encountered in all branches of chemistry, and a shared feature in all scenarios for abiogenesis. While formalizations exist for particular instances, autocatalysis in chemistry lacks a unifying framework that captures all reported autocatalysis, and unknown forms of autocatalysis may still have to be identified.

Here, we introduce this framework, by deriving general properties in chemical reaction networks for catalysis and autocatalysis that follow directly from basic definitions in chemistry. These definitions imply minimal structural motifs in autocatalytic networks which come in five types, of which two have not yet been encountered. Branching processes allow to assess the kinetic viability of networks, which depends on such motifs. We further extend the range of conceivable autocatalysis by showing that autocatalytic motifs readily emerge in a multicompartment setting. Autocatalysis can thereby be realized from a single uncatalyzed chemical reaction, suggesting the phenomenon may in fact be widespread.

Blokhuis, Alex; Lacoste, David; Nghe, Philippe (2020): Autocatalysis in Chemical Networks: Unifications and Extensions. ChemRxiv.
Preprint. https://doi.org/10.26434/chemrxiv.12317273.v1
Blokhuis, Alex (2019); Physical Aspects of Origins of Life Scenarios. Thesis, PSL Research University, ESPCI. https://hal.archives-ouvertes.fr/tel-02566386/

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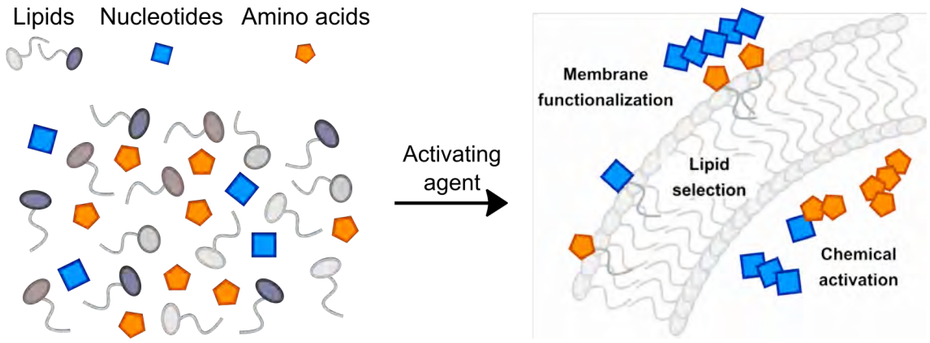

TOWARDS THE EMERGENCE OF MODERN CELL MEMBRANES

C. Bonfio, **J.D. Sutherland**
MRC Laboratory of Molecular Biology -Cambridge (United Kingdom)

The complexity of modern biochemistry suggests that a systems chemistry approach is requiredto understand and potentially recapitulate the intricate network of prebiotic reactions that led to theemergence of life. Early cells probably relied upon compatible and interconnected chemistries to linkRNA, peptides and membranes. In this context, understanding how and when phospholipid membranesappeared on early Earth is critical to elucidating the prebiotic pathways that led to the emergence ofprimitive cells. Starting with a mixture of activated carboxylic acids of different lengths, iterative cyclingof acylation and hydrolysis steps allowed for the selection of longer-chain acylglycerol-phosphatesthrough accumulation-induced compartmentalization of self-assembling amphiphiles at the expense ofnon-self-assembling shorter chain analogues. Our results suggest that a selection pathway based onenergy-dissipative cycling could have driven the selectivesynthesis of phospholipids on the early Earth[1].Moreover, I will show that several types of vesicles, formed from prebiotically plausiblemixtures of amphiphiles, allow activation of amino acids, peptides and nucleotides. Interestingly,activation chemistry drives the advantageous conversion of reactive amphiphiles into inertcyclophospholipids, thus supporting their potential role as major constituents of primitive cells.Activation of prebiotic building blocks within fatty acid-based vesicles yields lipidated species capable oflocalizing and functionalizing primitive membranes. Our findings describe a potentially prebioticnetwork of reactions in which the components of primitive cells could have selectively undergoneactivation and reacted to yield new species, which enabled the emergence of cells with increasinglyadvanced functionalities[2].

1 Bonfio C. et al., J. Am. Chem. Soc.2019, 141, 3934–3939.
2 Bonfio C. et al., submitted.

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FLOOR 4

THERMAL STABILITY OF METALORGANIC COMPOUNDS ON VOLCANIC OLIVINE

Joanna Brau[1], **Marco Matzka[2], Philippe Schmitt-Kopplin[2,3], Norbert Hertkorn[2], Werner Ertel-Ingrisch[1], Bettina Scheu[1], and Donald B. Dingwell[1]**
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[2] Helmholtz Zentrum München, Neuherberg, Germany;
[3] Technische Universität München, Freising, Germany

Previously unknown class of metalorganic compounds revealed in meteorites[1] also found on the surfaces of silicate phases such as olivine, may have been involved in the emergence of life. Here, the thermal stability of such organic compounds has been experimentally investigated under conditions which simulate those extant on the early Earth. We have studied olivines from the Hawaiian eruptions of 1959 and 2018. Individual mineral grains have been hand-picked to be free of secondary phases such as pyroxene or melt. We use a high temperature gas-tight tube furnace under CO-CO_2 gas mixture at temperatures ranging from 950°C to 1350°C and oxygen fugacity ranging from 10-12 bar, within the stability field of olivine. The samples were contained in Pt crucibles and held for dwell times of 1 to 8 h. Quenching was performed by lifting the samples vertically out of the tube furnace. Using EPMA (electron microprobe analyzer) and RAMAN spectroscopy, we have mapped the state of the olivine samples. We observe that the composition of the individual mineral grains remains stable and homogeneous with thermal treatment. The metalorganic cargo of these olivines has been analyzed using FT-ICR- MS (Fourier Transform ion cyclotron mass spectrometry). Preliminary results reveal systematic changes or organic molecular composition depending on time and heat of thermal treatment whose origins will be discussed..

1 A. Ruf, B. Kanawati, N. Hertkorn, Q. Yin, F. Moritz, M. Harir, M. Lucio, B. Michalke, J. Wimpenny, S. Shilobreeva, B. Bronsky, V. Saraykin, Z. Gabelica, R. D. Gougeon, E. Quirico, S. Ralew, T. Jakubowski, H. Haack, M. Gonsior, P. Jenniskens, N. W. Hinman, P. Schmitt-Kopplin. Previously unknown class of metalorganic compounds revealed in meteorites. PNAS 114 (2017) 2819-2824.

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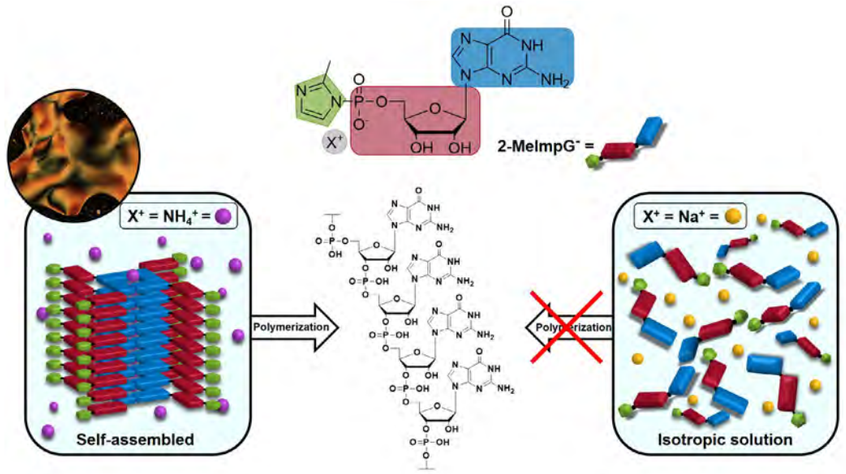

SELF-ASSEMBLY DRIVEN POLYMERIZATION OF ACTIVATED NUCLEOTIDES

Federico Caimi[1], **Marco Todisco[1], Diego Colombo[1], Sara Sattin[2], Tommaso Bellini[1]**

[1] Dipartimento di Biotecnologie Mediche e Medicina Traslazionale, Università degli Studi di Milano, via Vanvitelli 32, 20129 Milano, Italy

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One of the most mind-bending problems about the "RNA World" hypothesis is the lack of a process to explain the ligation of monomeric nucleotides into linear chains.

Many mechanisms for the abiotic polymerization have been proposed, but no one without issues. Among them phosphoroimidazolides, carrying the energy required to form phosphodiester bonds, can perform the nonenzymatic copying of RNA templates.[1] However, this process relies on the presence of a preformed RNA chain to drive the polymerization, favoring the reactivity and preventing the formation of cyclic products.

It has been recently discovered that nucleic acids, at high concentration, can self-assemble into linear aggregates[2], that in turn enhance their chance of ligating when in the presence of condensing agents like carbodiimides.[3]

Here we report that imidazole-activated guanosines can self-assemble forming G-quadruplex columns and order into nematic liquid crystal phases, analogously to guanosine monophosphate. These columns are formed by stacked tetrads of Hoogsteen-paired guanines, which resemble the secondary structures found in guanine-rich DNA and RNA strands. We find that the organization provided by these structures drives, without the need of templating strands, the polymerization of phosphoroimidazolides into oligos limited in length by the peculiar reaction mechanism of these molecules.

With a simple simulation we find that in a static structure the polymerization can run into some breakpoints hampering the formation of longer oligos.

To introduce some dynamics to the system we designed some wet-dry cycles adding fresh activated nucleotide to each cycle increasing the polymerization up to decamers.

By demonstrating a path of polymerization through self-assembly, our findings support the idea of a primeval world in which RNA strands emerged from pools of self-assembled molecules.

1 J. Am. Chem. Soc. 2016, 138, 11996–12002
2 PNAS 2008, 105 (4), 1111-7
3 ACS Nano 2018 12 (10), 9750-9762

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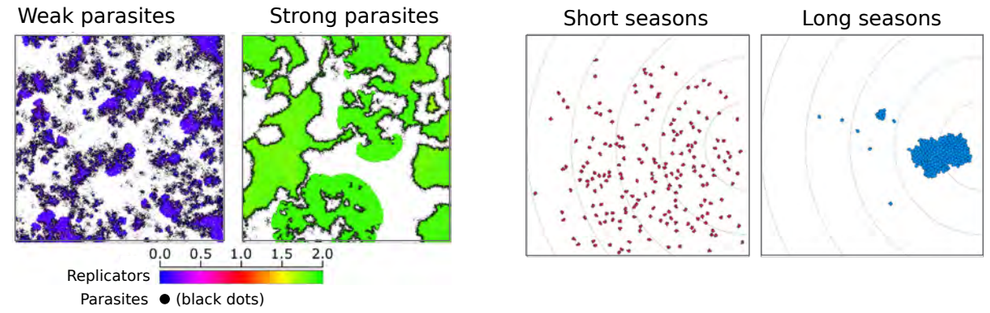

EMERGENCE OF NOVELTY AND EVOLUTIONARY TRANSITIONS

Enrico Sandro Colizzi
Leiden University, Origins Center

Novel functions and traits have appeared throughout the four billion years of evolutionary history. The emergence of novelty is particularly salient during Major Evolutionary Transitions - where new levels of individuality are generated by the self-organisation of its constituting components - because entire new spaces of possibilities are opened. Evolutionary novelty is typically understood "a posteriori" by tracing back the steps that generated it.

I show that novelty can be understood - by mathematical modelling - also without presuming the result. I present two very different models, one about the Origin of Life and the other about the Evolution of Multicellular Life, and show that novelty arises in a similar way.

In the Origin of Life model, RNA-like replicators can evolve the degree to which they replicate one another. In the Origin of Multicellularity model, cells follow a noisy signal that lead to resources, and can evolve the degree to which they stick to each other. In both models, the self-organisation of replicators (RNAs or cells) into higher-level individuals (RNA replicator-parasite waves or multicellular organisms) create functional properties that did not exist outside of the higher-level context (hence novel) and that profoundly affect the evolutionary dynamics of the replicators.

In conclusion, the interplay between self-organisation and evolution readily generates novelty.

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TRACING PRIMORDIAL METABOLISM REFLECTED BY MICROORGANISMS UNDER HYDROTHERMAL CONDITIONS

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[1] Department of Earth and Environmental Sciences, Ludwig-Maximilians Universität, 80333 Munich, Germany
[2] Chair of Biochemistry, Department of Chemistry, Technische Universität München, Garching, Germany
[3] GeoBio-CenterLMU, Ludwig-Maximilians Universität, 80333 Munich, Germany

The origin of life is hypothesized to be linked to autocatalytic carbon fixation pathways under primordial hydrothermal conditions[1].
The main goal of this project is to provide experimental, field, and theoretical constraints on the functioning and evolution of carbon fixation pathways while combining microbiology and chemistry.
Using isotopologue profiling analysis, we investigate carbon fixation in different heterotropic and autotrophic model organisms, namely Bacillus subtilis[2], Hippea maritima, Pyrobaculum arsenaticum and Raoultella planticola. These data will be compared to microbial communities expressing the rTCA and reductive acetyl-CoA pathways sampled from Loki's castle in collaboration with Bergen University, active volcanism driven hydrothermal area in Milos (in collaboration with Bergen University) and geothermal springs/wells in Eastern Anatolia in Turkey (in collaboration with Istanbul University). Twenty good to high quality metagenomic bins were constructed from samples taken from the Turkey and three bins affiliated to deeply branching hydrogen oxidizing Aquificae were found. Further evaluation on metagenomic bins, future fieldworks and metatransciptomic studies of hydrothermal samples will validate the experimental results under natural conditions, by assessing how natural hydrothermal settings can favor the expression of either pathway or pathway components. Our project will result in novel insights into early metabolic evolution under hydrothermal conditions.

1 Fuchs, G. Alternative pathways of carbon dioxide fixation: insights into the early evolution of life? Annu Rev Microbiol 65, 631-658, doi:10.1146/annurev-micro-090110-102801 (2011).
2 Spona-Friedl M. Substrate-dependent CO2-fixation in heterotrophic bacteria revealed by stable isotope labelling FEMS Microbiol Ecol 96, fiaa080, doi: 10.1093/femsec/fiaa080 (2020).

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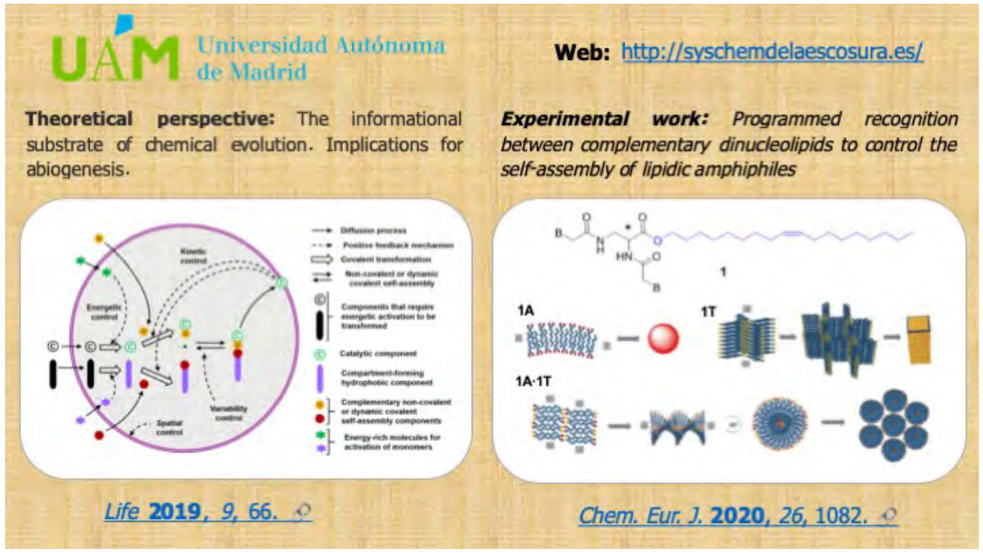

BIOHYBRID MATERIALS AND SYSTEMS CHEMISTRY

Andres de la Escosura[1,2], **Sonia Vela-Gallego[1], Stefania Kalantzi[1], Noemi Nogal-Rodriguez[1], Santiago Guisan[1]**

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[2] Institute for Advanced Research in Chemistry (IAdChem), Campus de Cantoblanco 28049, Madrid, Spain.

The study of complex molecular networks and supramolecular assemblies is a clear objective of the field so-called systems chemistry, which is expected to have a great impact in the area of origins-of-life research and as biohybrid materials in materials science. With regards to the origins of life, a pertinent question is whether artificial cells could be constructed from non-natural components. In order to provide clues about this question, we have started research lines on nucleic acid hybrids and nucleolipid compartments. The study and combination of these components is an interesting approach because it allows exploring some properties of life without the restrictions of the historical pathway that Darwinian evolution took. Concerning the approach to biohybrid materials, we focus our work on supramolecular biohybrids for biomedical light management, which combine different photoactive molecules with peptide, protein and nucleic acid nanostructures. In this poster presentation we will shortly discuss some of these research lines.

S. Morales-Reina, C. Giri, M. Leclercq, S. Vela-Gallego, I. de la Torre, J. R. Caston, M. Surin, A. de la Escosura, 2020. "Programmed Recognition Between Complementary Dinucleolipids to Control the Self-Assembly of Lipidic Amphiphiles", Chem. Eur. J., 26, 1082.
A. de la Escosura, 2019. "The Informational Substrate of Chemical Evolution: Impli-cations for Abiogenesis", Life, 9, 66.
V. Almeida-Marrero, E. van de Winckle, E. Anaya-Plaza, T. Torres, A. de la Escosura, 2018. "Porphyrinoid Biohybrid Materials as an Emerging Toolbox for Biomedical Light Management", Chem. Soc. Rev., 47, 19.
K. Ruiz-Mirazo, C. Briones, A. de la Escosura, 2017. "Chemical Roots of Biological Evolution: The Origins of Life as a Process of Development of Autonomous Functional Systems", Open Biol. 7, 170050.
K. Ruiz-Mirazo, C. Briones, A. de la Escosura, 2014. "Prebiotic Systems Chemistry: New Perspectives for the Origins of Life", Chem. Rev. 114, 285-366.

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ANOMALOUS FLUCTUATIONS AND SELECTIVE EXTINCTION IN PRIMORDIAL REPLICATORS: A "STRUGGLE FOR LIFE" AT THE ORIGIN OF BIOLOGICAL CHIRALITY

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[1] Department of Chemistry – Università degli Studi di Bari Aldo Moro – Via Orabona 4 – 70125 Bari, Italy

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[3] Istituto per la Scienza e Tecnologia dei Plasmi – Consiglio Nazionale delle Ricerche, Bari Section – Via Amendola 122/D – 70125 Bari, Italy

One of the most distinctive signs of life as we know it, is the presence of a single chiral variant in living organisms and one of the greatest ambitions for biochemistry and astrobiology is to provide an explanation of this predominance. Several mechanisms were proposed in the past, here we propose a different scenario: anomalous fluctuations associated with a self-replication process can lead to selective extinction of one of the two variants. The idea is based on three key-points: a) the simulation of early biological processes as a "board game"; b) the presence of large fluctuations during an autocatalytic process; c) the presence of a limited source of chemical energy, inducing a form of competition in a primordial replicator population. In order to demonstrate this mechanism, a computational model is developed, describing the "struggle for life" of two different kinds of primordial replicators on a "chessboard" with periodic boundary conditions. Each replicator employs enzymes of different chirality on a non-chiral substrate. The replication occurs randomly and with a fixed probability, providing that a sufficient amount of chemical energy is locally available. Results clearly show that strong fluctuations in the number of individuals of each species and a subsequent selective extinction of one of the two are observed. In the next step of our research, a more structured variant of the mechanism will be considered. This will concern experimental simulations with more complicated assumptions. More complex organisms and biological behavior will be investigated. Phenotypes, potentially favorable in the "struggle for life" will be introduced. Phenotypes are acquired on the basis of a genotype; therefore, our model will be implemented with a genetic code which could be inherited or even mutated producing different phenotypes. These studies may contribute to shed light on the transition occurred during the biochemical evolution of our planet.

Longo, S. (2019). Anomalous fluctuations and selective extinction in populations of primordial, EANA 2019, Orléans

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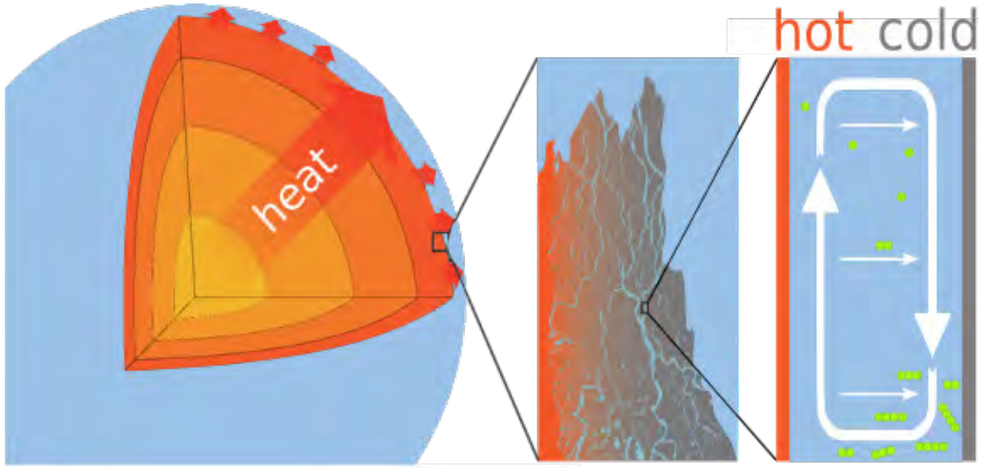

ESCALATION OF DNA MONOMER POLYMERIZATION IN THERMAL TRAPS

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Highly diluted starting concentrations and the 'tyranny of the shortest' are the main problems for de novo strand formation of DNA/RNA on Early Earth. A possible scenario that could have overcome these issues are thermogravitational traps in hydrothermal vent systems[1]. We demonstrate that these traps can accumulate solutions of single molecules despite their high diffusivity. We prove that there are non-enzymatic chemistries that are designed to polymerize RNA also polymerize DNA mononucleotides. However, the concentrations of the strands decrease exponentially with length leaving the long strands to be the inferior species. In non-equilibrium conditions provided by thermogravitational traps an accumulation of DNA strands is taking place that is exponentially length dependent[2]. We show that the trapping procedure significantly increases the probability that longer strands are linked together and consequently leads to an escalation of DNA polymerization. If additionally, two complementary monomers are present in the system, self-templated ligation can take place after the first spontaneous formation of oligomers.

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2 Escalation of polymerization in a thermal gradient. C.B. Mast, S. Schink, U. Gerland & D. Braun. PNAS 110,8030-8035 (2013)

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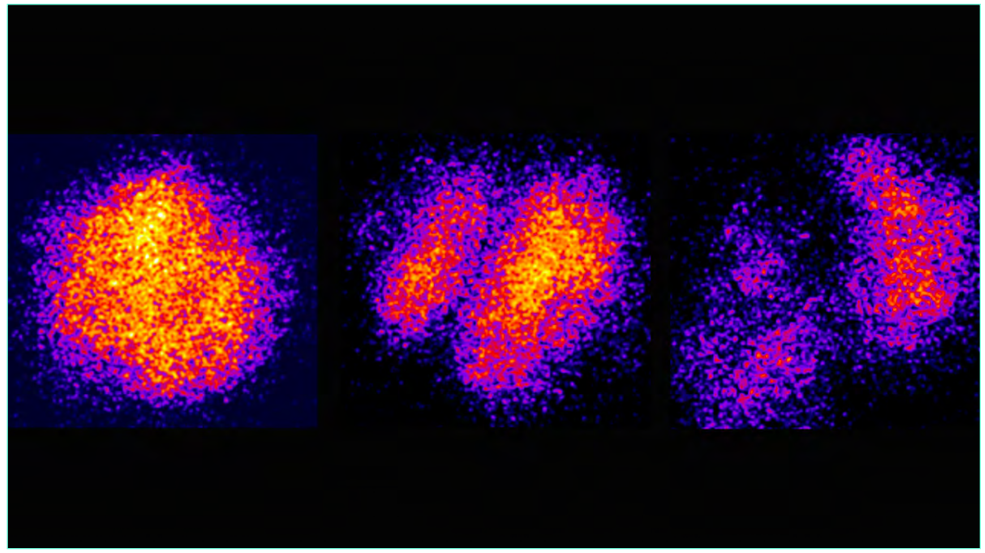

ACTIVE COACERVATE DROPLETS AS A PLATFORM TOWARDS SYNTHETIC LIFE

Carsten Donau[1], Fabian Spaeth[1], Marilyne Sosson[1], Brigitte Kriebisch[1], Fabian Schnitter[1], Marta Tena-Solsona[1,2], Hyun-Seo Kang[1,3], Elia Salibi[4], Michael Sattler[1,3], Hannes Mutschler[4], Job Boekhoven[1,2]
[1] Department of Chemistry, Technical University of Munich, Lichtenbergstrasse 4, 85748 Garching, Germany
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Membraneless organelles like stress granules are active liquid-liquid phase-separated droplets that are involved in many intracellular processes. Their active and dynamic behavior is often regulated by ATP-dependent reactions. However, how exactly membraneless organelles control their dynamic composition remains poorly understood. Herein[1], we present a model for membraneless organelles based on RNA-containing active coacervate droplets regulated by a fuel-driven reaction cycle. These droplets emerge when fuel is present, but decay without. Moreover, we find these droplets can transiently up-concentrate functional RNA, and that this up-take is accelerated by the chemical reaction cycle. Finally, we show that in their pathway towards decay, these droplets self-divide asymmetri-cally. Self-division combined with emergence, decay, rapid exchange of building blocks, and functionality are all hallmarks of life, and we believe that our work could be a stepping stone towards its synthesis.

1 ChemRXiv: “Active Coacervate Droplets as a Model for Membraneless Orga-nelles and a Platform Towards Synthetic Life“

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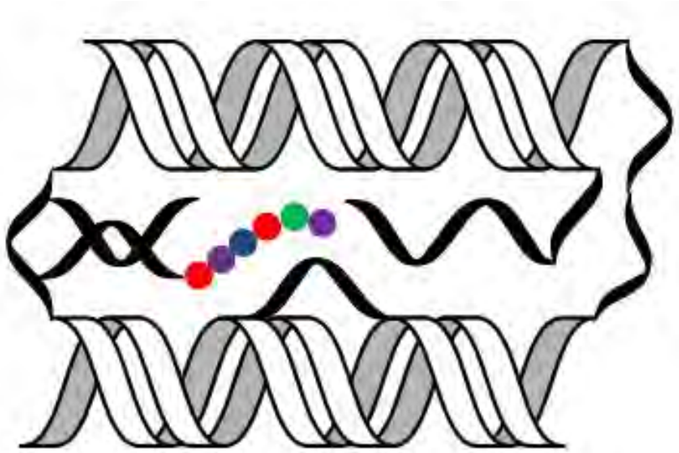

OLIGONUCLEOTIDE ASSEMBLIES AS EARLY RIBOSOMES

Olivia Doppleb[1], **Arthur Ermatov[2], Biswarup Jash[1], Rainer-Joachim Schwarz[1], Tim Liedl[2], Clemens Richert[1]**
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As Francis Crick et al. wrote, "The origin of protein synthesis is a notoriously difficult problem. We do not mean by this the formation of random polypeptides but the origin of the synthesis of polypeptides directed, however crudely, by a nucleic acid template and of such a nature that it could evolve by steps into the present genetic code."[1] This difficult problem is still unsolved.[2] The earliest organisms capable of RNA-induced peptide synthesis must have possessed a much simpler form of molecular machinery than the ribosomal apparatus. Based on the experimental observation of unencoded formation of 'peptido RNA' from amino acids and nucleotides in condensation buffer[3,4], we are studying the effect of multistrand assemblies on the nanometer scale on peptide and peptido RNA formation. This includes assemblies with RNA primers that possess binding pockets for amino acids and templated reactions with tRNAs.[5]
In particular, we are investigating reactions in small folded DNA or RNA structures comprising 65 base pairs or less and gaps of one or two nucleotides. Such assemblies can have a profound effect on peptide chain growth in aqueous condensation buffers.

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TRACKING LIFE AT THE BREAK OF DAWN- IDENTIFICATION & INTERPRETATION OF BIOSIGNATURES IN EARTH'S OLDEST ROCKS

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[3] Linnaeus University, Kalmar, Sweden

When and under what conditions did life emerge? The geological record holds detailed information relevant to these questions. Particularly important are geologically stable signatures that can be used to track primordial life and, potentially, provide information on its nature (i.e., biosignatures). However, the identification of unequivocal biosignatures in Earth's oldest rocks is incredibly challenging. For instance, candidate signatures must be demonstrably syngenetic with the formation of the host rock and assuredly be of biological origin. Once established, the interpretation of biosignatures is a further challenge we face. This is because biological processes are extremely complex, and so are the resulting signatures. In this presentation, we will demonstrate how we can yet extract valuable information from the geological record by combining field observations with a variety of rock-based approaches (e.g., analytical imaging techniques, organic-geochemical analyses)[1,2]. Furthermore, we will show how we can use younger analogue systems (e.g., hydrothermal Lake Magadi, Kenya[3]) and laboratory experiments (e.g., Fischer–Tropsch-type synthesis of organic matter[4]) to fill remaining gaps in understanding. This integrative approach has allowed us to successfully identify and interpret unequivocal biosignatures in some of Earth's oldest rocks (e.g., 3.4-Byr-old mineralized microbial mats1, 3.5-Byr-old organic biomolecules2). Furthermore, it has provided detailed insights into the nature of early Earth's habitats. In the long run, our studies will help to develop a solid understanding of how life emerged on our planet (and possibly beyond)..

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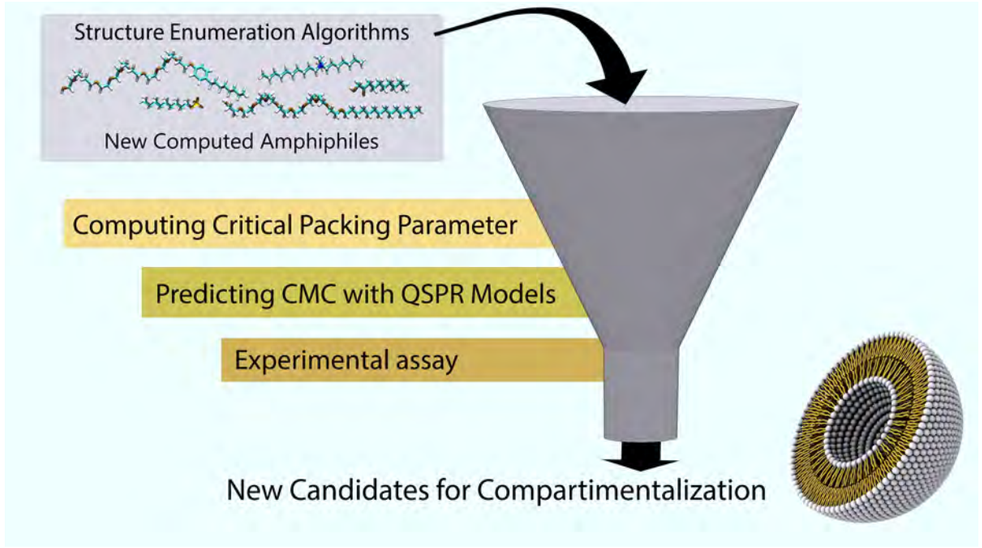

COMPUTATIONAL EXPLORATION OF LIPID CHEMICAL SPACE : PREDICTING ASSEMBLY USING QSPR MODELS

Selene Forget, **Ric Gillams, Tony Jia**
Markus Meringer, **Jim Cleaves**
Ecole Normale Supérieure

Compartmentalization is likely to have been essential for the emergence of life. Compartmentalization allows for the creation of unique chemical conditions that can be maintained out of equilibrium with the environment and the exclusion of parasites. Confining organic molecules also helps limit diffusion, increases concentration and can thus influence both the thermodynamics and kinetics of prebiotic reactions. Biology currently predominantly uses phospholipids to construct cell membranes. However, there are many other types of organic compounds that can form stable compartments in water, and many of these may have been abundant in the prebiotic environment. In this study we explore this alternative lipid chemical space by using structure enumeration algorithms to compute an exhaustive combinatorial library of surfactant molecules. We then predict the propensity of these compounds to self-assemble into membranes using quantitative structure-property relationship (QSPR) models on critical micelle concentration (CMC). Combined with critical packing parameter calculations, these models can allow identification of novel molecule types which can be experimentally assayed as candidates for the emergence of protocells.

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LIQUID CRYSTAL COACERVATES: A PATHWAY FOR BIO-POLYMERS COEVOLUTION AND COMPLEX PROTO-CELLULAR STRUCTURING

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The abiotic formation of biopolymers from their monomeric building blocks and the emergence of cellular structure are still unsolved problems in the origin of life investigation.
Here we report the formation of liquid crystal phases inside complex coacervate microdroplets in mixtures of short dsDNA and cationic peptides[1]. This system reveals a much more complex phase diagram than normal unstructured coacervates and reversibly transitions between each phase state with continuity upon variations in temperature and added salt, DNA and peptide concentration.
Coacervation decreases the global dsDNA concentration required for the nucleation of all LC mesophases previously observed in bulk[2].
Remarkably and counterintuitively, in drying-wetting cycles, this system can escape precipitation simply by drying, and accesses ordered, yet fluid, phases by dilution of a homogeneous liquid phase.
Additionally, we show that the dense coacervate phase enhances the rate of non-enzymatic ligation reactions, resulting in the elongation of constituent short dsDNA up to more than 10 times their initial length, while the reaction is ineffective in the diluted phase.
The cooperative assembly of nucleic acids monomers[3] and oligomeric peptides templated by LC ordering inside the coacervate phase can constitute a pathway for the formation and co-evolution of life polymers. LC-coacervates can generate multi-phase compartments with different degrees of order[4] and permeability to guest molecules, which can result in effective and structured model protocells.

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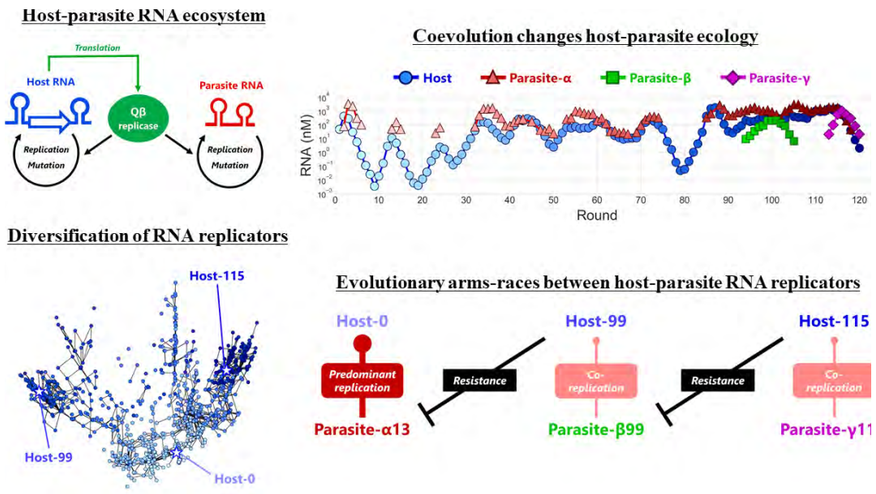

EMERGENCE AND DIVERSIFICATION OF A HOST-PARASITE RNA ECOSYSTEM THROUGH DARWINIAN EVOLUTION

Taro Furubayashi[1], Kensuke Ueda[2], Yohsuke Bansho[3], Daisuke Motooka[4], Shota Nakamura[4], Ryo Mizuuchi[5,6], Norikazu Ichihashi[2,3,5,7,8]

[1] Laboratoire Gulliver, CNRS, ESPCI Paris, PSL Research University, Paris, France
[2] Department of Bioinformatic Engineering, Graduate School of Information Science and Technology, Osaka University, Osaka, Japan
[3] Graduate School of Frontier Biosciences, Osaka University, Osaka, Japan
[4] Research Institute for Microbial Diseases, Osaka University, Osaka, Japan
[5] Komaba Institute for Science, The University of Tokyo, Tokyo, Japan
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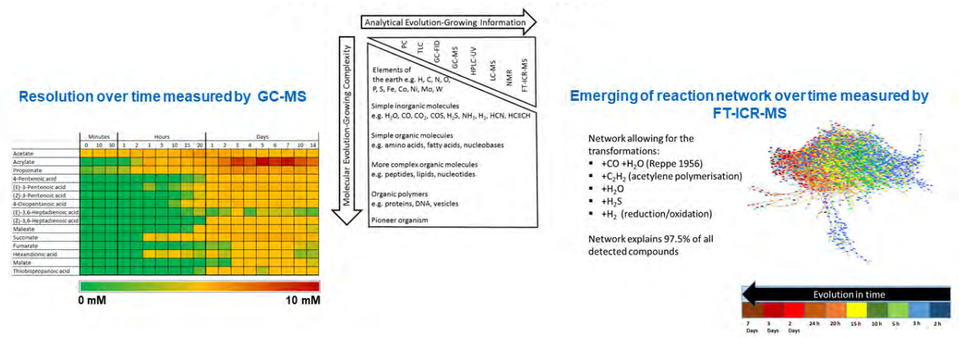
In prebiotic evolution, molecular self-replicators are considered to develop into diverse, complex living organisms. The appearance of parasitic replicators is believed inevitable in this process. However, the role of parasitic replicators in prebiotic evolution remains elusive. Here, we demonstrated experimental coevolution of RNA self-replicators (host RNAs) and emerging parasitic replicators (parasitic RNAs) using an RNA-protein replication system we developed. During a long-term replication experiment, a clonal population of the host RNA turned into an evolving host-parasite ecosystem through the continuous emergence of new types of host and parasitic RNAs produced by replication errors. The host and parasitic RNAs diversified into at least two and three different lineages, respectively, and they exhibited evolutionary arms-race dynamics. The parasitic RNA accumulated unique mutations, thus adding a new genetic variation to the whole replicator ensemble. These results provide the first experimental evidence that the coevolutionary interplay between host-parasite molecules plays a key role in generating diversity and complexity in prebiotic molecular evolution.



CHEMICAL EVOLUTION OF BIOMOLECULES FORMED UNDER VOLCANIC HYDRO-THERMAL CONDITIONS

Thomas Geisberger[1], Philippe Diederich[2], Claudia Huber[1] and Philippe Schmitt-Kopplin[2]

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[2] Research Unit Analytical Biogeochemistry, HelmholtzZentrum München

Reactions mimicking volcanic-hydrothermal vent conditions are performed. Main group volatiles (e.g. CO_2, CO, COS, HCN, C_2H_2, H_2S, N_2, H_2, NH_3, HCN, P_4O_{10}) in aqueous solution react on the surfaces of crustal catalytic transition metal minerals (e.g. FeS, NiS, CoS)[1]. The basic setup of the experiment consists of NiS in water under an acetylene and carbon monoxide atmosphere. The mixture is kept at 378 K for several hours and the temporal evolution of the reaction mixture was monitored. Later experiments added NH_3 to the system. In addition to previously established GC/MS analysis, the combination of high-resolving analytical tools[2,3] and data-analytical approaches[4] will enable us to decipher the complex reaction mixtures. Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS), gas chromatography-MS (GC-MS) and nuclear magnetic resonance (NMR) methods provide complementary profiles of the complex product mixtures for both low and high molecular weight compounds, including a remarkable variety of CHOS derivatives.

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SELECTION PRESSURE: THE LATITUDINAL BIODIVERSITY GRADIENT IS DRIVEN BY THE LATITUDINAL VARIATION OF ULTRAVIOLET RADIATION

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The fundamental principle of life is Darwinian evolution. Ultraviolet radiation is a known mutagen and a factor for selection pressure on Earth's prebiotics. Ultraviolet irradiance peaks at the tropics and minimises at the poles. Species richness also peaks at the tropics and minimises at the poles. Previous literature reviews hypothesise that increased biomass and species richness at the tropics might be caused by the solar energy presence, but the mechanism is unclear. In this study, the role of latitudinal variation of ultraviolet irradiance on the latitudinal biodiversity gradient is investigated. A mathematical relation between latitudinal biodiversity gradient and latitudinal variation of ultraviolet radiation is discussed. The preliminary approach shows that the latitudinal biodiversity gradient might be driven by the latitudinal variation of ultraviolet radiation.

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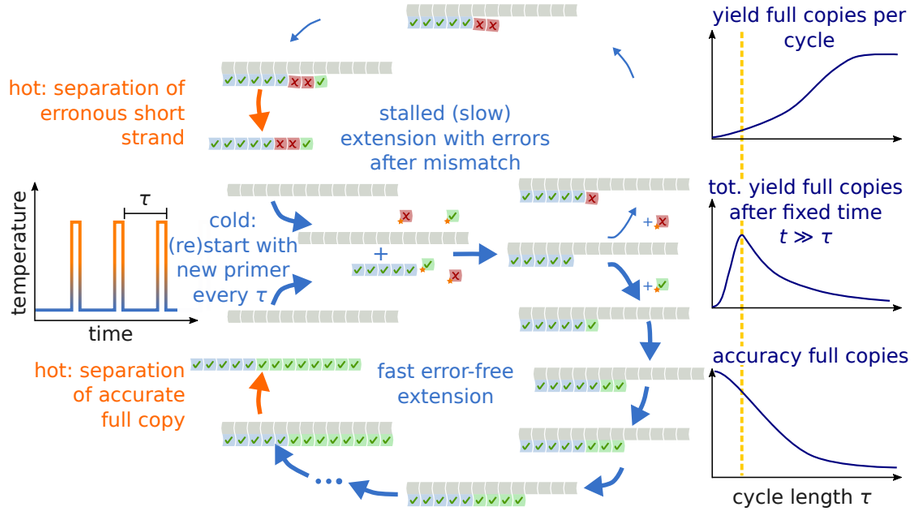

A NONEQUILIBRIUM ERROR FILTERING MECHANISM FOR ENZYME-FREE COPYING OF NUCLEIC ACID SEQUENCES

Tobias Göppel[1], **Benedikt Obermayer[2], Joachim Rosenberger[1], Bernhard Altaner[1], Gabrielle Leveau[3], Clemens Richert[3], Irene Chen[4], and Ulrich Gerland[1]**

[1] Physics of Complex Biosystems, Physics Department, Technical University of Munich, James-Franck-Str. 1, D-85748 Garching, Germany
[2] Systems Biology of Gene Regulatory Elements, Berlin Institute for Medical Systems Biology, Max Delbrück Center for Molecular Medicine in the Helmholtz Association, Robert-Rössle-Straße 10, D-13125 Berlin, Germany; Core Unit Bioinformatics, Berlin Institute of Health, Charité - Universitätsmedizin Berlin, Charit latz 1, D-10117 Berlin, Germany.
[3]Institute of Organic Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany
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Accurate copying of nucleic acid sequences by template-directed polymerization is essential for self-replicating and evolving systems. Modern cells achieve error rates as low as 10−9 with sophisticated enzymatic machineries that consume free energy to repeatedly discriminate between correct and incorrect nucleotides. In contrast, experiments probing template-directed, nonenzymatic extension of RNA and DNA as potential prebiotic copying processes find error rates of roughly 10−1, making it impossible to reliably transmit information from one strand generation to another. However, it is observed that initial incorporation errors trigger a cascade of consecutive errors and significantly reduce the speed of downstream extension, an effect called stalling. This phenomenon opens the door to an early error reduction mechanism: Using computer simulations and mathematical modelling, we show that error cascades can be exploited to discriminate between faithful and faulty polymerization products by means of their global kinetics. Limiting the time window for the polymerization process prevents erroneous strands to complete resulting in a pool where full-length products show an enhanced accuracy. Such a mechanism does not require any additional energy input to the extension reaction itself and can be controlled externally. However, filtering out strands is at the expense of the overall yield and hence a characterization of the fidelity-yield trade-off is needed. The yield problem can be circumvented though a repeated copying process where a strand serves as a template multiple times. Such a process may be induced by temperature cycles occurring naturally in the vicinity of hydrothermal vents which were common on the early Earth.

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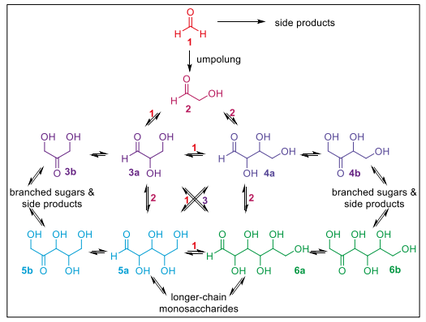
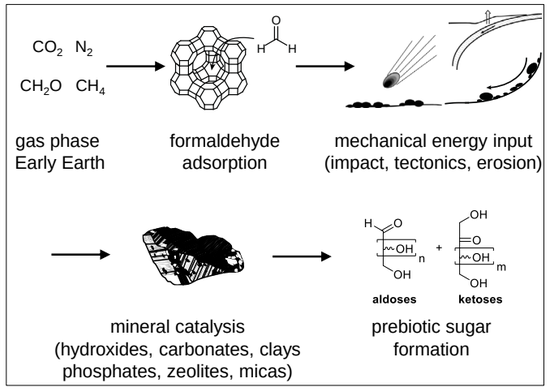
Formose Reaction



Mechanochemistry as a scenario for the Early Earth



A MINERAL-CATALYSED, MECHANOCHEMICAL FORMOSE REACTION

Maren Haas[1,2], Saskia Lamour[1,2], Sarah B. Christ[2], Oliver Trapp[1,2]

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The formose reaction builds up monosaccharides from formaldehyde and glycolaldehyde and a basic catalyst and is one of the possible formation pathways for carbohydrates on the Early Earth.[1,2] However, it suffers from side reactions and deterioration of the products under the highly alkaline reaction conditions.[3]

Most of the postulated scenarios for prebiotic reactions are based on aqueous reaction media like the “warm little pond” or hydrothermal vents.[4] Solvent-free reactions represent an alternative setting for prebiotic reactions and can be accelerated by mechanic energy inputs like lithospheric activity, weathering, erosion, diagenesis, tectonics or meteor impacts. Under laboratory conditions ball mills are used for the investigation of mechanochemical reactions.

We present the combination of the formose reaction and the mechanochemical setting in the context of the origins of life.

The formation of carbohydrates by ball milling formaldehyde and glycolaldehyde with mineral catalysts is observed.[5] These reactions gain from higher selectivity and decreased decomposition in comparison to the aqueous reaction. Two-step derivatization and subsequent analysis by gas chromato¬graphy-mass spectrometry is used to investigate the formed reaction mixtures.[6]

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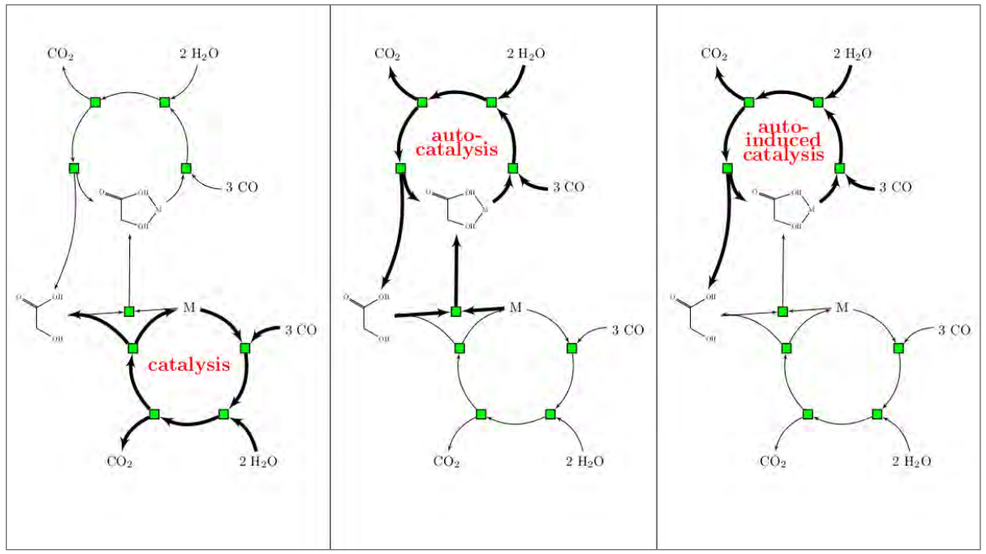

IDENTIFICATION OF AUTOCATALYSIS IN A REACTION NETWORK - A GRAPH-TOPOLOGICAL APPROACH

Philipp Honegger[1] **and Christoph Flamm**[2]

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The concept of autocatalysis refers to a chemical reaction producing copies of its catalyst. Autocatalysis is indispensible to abiogenetical questions due to the ability of such systems to feed on input molecules, grow and reproduce. Autocatalytic species possess the necessary robustness against environmental shocks and continuous molecular degradation,[1] and they allow for the emergence of enantiomeric excesses ex nihilo by ampliying statistical fluctuations of enantiomer ratios.[2,3] Even evolved modern-day metabolisms are suspected to contain ancestral autocatalytic cores.[4]

We present the structural requirements autocatalysis imposes on the underlying chemical reaction networks and show examples from chemistry and biology. This permits the comprehensive detection of possible autocatalytic reactions. In this context, we also show its reverse counterpart, destructive autocatalysis. Reverse-autocatalytic motifs present in the reaction network are able to counteract productive autocatalytic cycles.

Our graph-topological analysis also differentiates between autocatalysis and autoinduction. The latter refers to chemical reactions where a product enhances the reaction rate of its production without producing more catalyst, for instance by starting material activation. Autoinductive reactions can exhibit similar kinetic signatures, but they do not possess the persistence aspect that distinguishes autocatalysis from common catalysis.[1]

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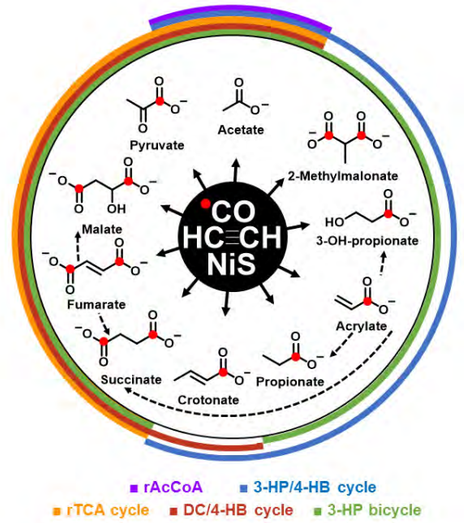

TOWARDS A POSSIBLE ACETYLENO/ CARBOXYDOTROPHIC CORE METABOLISM UNDER PRIMORDIAL CONDITIONS

Thomas Geisberger[1], **Jessica Sobotta**[1],**Thomas Steiner**[1], **Christian Seitz**[1], **Günter Wächtershäuser**[2], **Wolfgang Eisenreich**[1], **Claudia Huber**[1]

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Theories concerning the origin and early evolution of life have to consider carbon fixation as well as the evolution of metabolism. The extant biosphere owes its existence mainly to CO_2-fixation. Due to the low reactivity of CO_2, alternative geochemically available carbon sources should be considered. Acetylene (C_2H_2) and carbon monoxide (CO) can be found in hydrothermal exhalations[1,2] and iron-nickel-sulfides were present in early earth´s crust[3]. We could show a one-pot carbon fixation of acetylene and carbon monoxide by aqueous nickel sulfide (NiS) under hydrothermal (>100ºC) conditions[4]. We found more than ten key $C_{2\text{-}4}$ constituents of the extant four central CO_2-fixation cycles of the domains Bacteria and Archaea[5-7]. Some of the organic products engage in the same interconversions as seen in the extant central CO_2-fixation cycles. A primordial, non-cyclic acetyleno/carboxydotrophic metabolism is suggested. It is based on aqueous organo-metal chemistry, from which the extant central CO_2-fixation cycles based on thioester chemistry would have evolved by piecemeal modifications.

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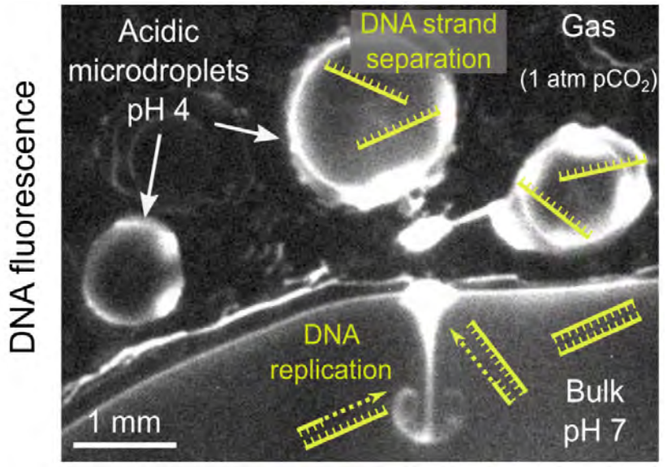

HEATED MICRODROPLETS OF ACIDIC WATER INDUCE THE DENATURATION OF OLIGONUCLEOTIDES AND THE REPLICATION OF LONGER STRANDS

Alan Ianeselli[1,2], **Miguel Atienza Juanatey[1], Christof B. Mast[1,2] and Dieter Braun[1,2]**
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The understanding of how the replication and the evolution of DNA or RNA sequences could have occurred on the primordial Earth is still an open debate in the Origin of Life community. Paradigms like Spiegelman's "tyranny of the shortest"[1] and the "strand separation problem"[2] are still some of the major barriers that most of the current models are not able to surpass. In this work, we created a prebiotically plausible physical system that tackles the aforementioned problems and could host the replication and the evolution of oligonucleotides autonomously. Our system consists of a thermal gradient across a rock pore containing liquid and gas enriched in CO_2. It periodically generated acidic microdroplets of condensation water that denatured DNA and RNA duplexes at moderate temperatures. At the same time, oligonucleotides of increasing length were accumulated at the gas-water boundaries and were preferentially denatured. The system was able to host enzymatic DNA replication at temperatures lower than the melting temperature and promoted the replication of longer sequences, avoiding the dominance of the shorter sequences in the pool.

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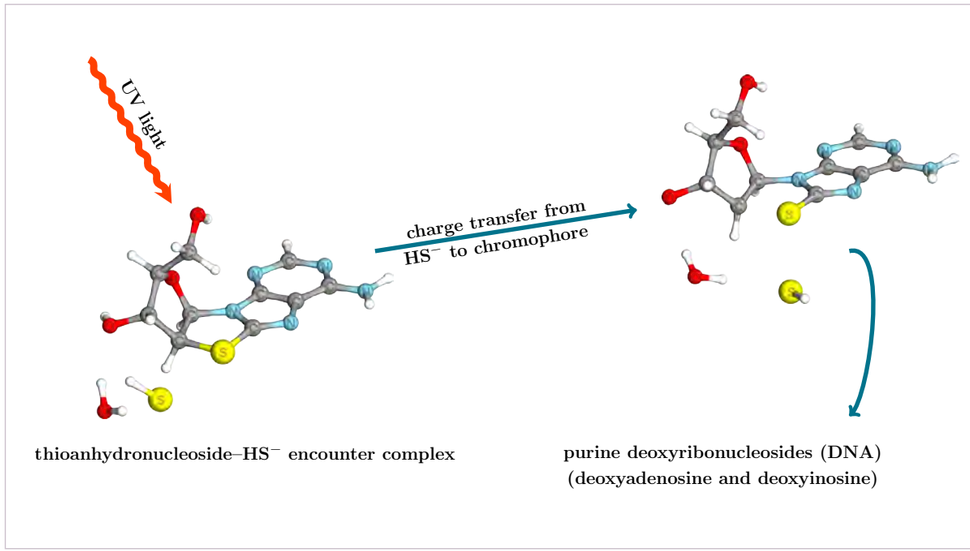

PHOTOREDUCTION OF THIOANHYDROADENOSINE TO THE PURINE DEOXYRIBONUCLEOSIDES

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In recent decades, a lot of efforts have been put into the exploration of abiotic synthesis of RNA and DNA nucleosides from prebiotically plausible feedstock molecules. Substantial progress has been made in the prebiotic synthesis of pyrimidine ribonucleosides. Despite many attempts, the abiotic synthetic routes towards DNA molecules, under the credible geochemical scenario, have not been found so far. The available results seem to support the RNA world hypothesis assuming RNA molecule could have been the first genetic polymer at the primordial Earth.[1] Furthermore, in this scenario, DNA polymer is appearing at a later stage of the development of early life. Our collaborative research performed with prof. John Sutherland's group enabled to discover the selective prebiotic synthesis of the purine deoxyribonucleosides showing that RNA and DNA may have coexisted at the origins of life.[2] Photoreduction of thioanhydroadenosine plays a key role in the newly uncovered prebiotic route to deoxyribonucleosides. To explain the mechanisms underlying photoreduction of thioanhydronucleosides, we performed quantum-chemical calculations of the excited-state potential energy surfaces to provide a mechanistic rationale for the UV-driven chemical reaction.

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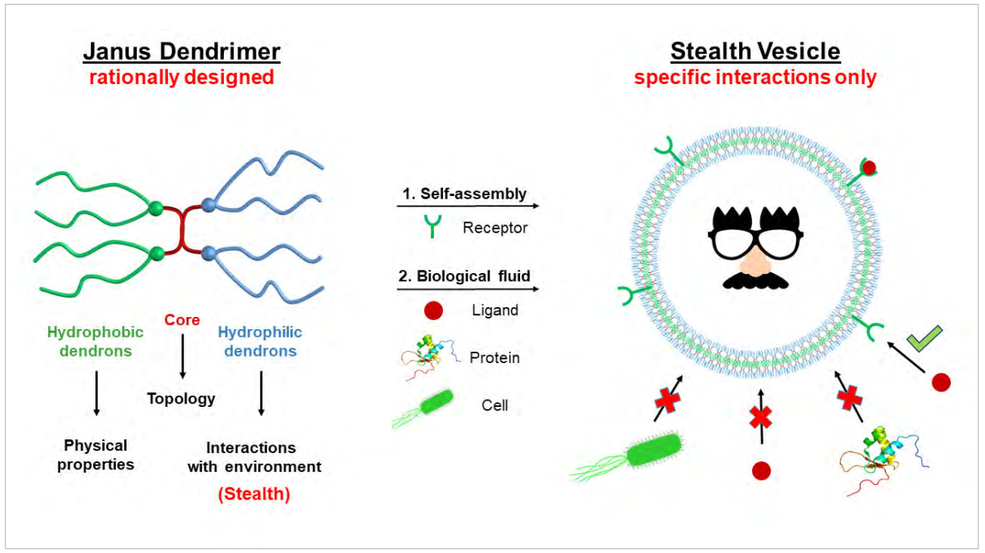

DESIGN OF STEALTH CELL-MIMETIC DENDRIMERSOMES

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The development of bottom-up synthetic cells requires the implementation of receptors into their membrane while the rest of the vesicle surface should be repellent towards non-specific adsorptions of proteins, sugars and cells. The current gold standards for stealth vesicle are co-assembled from natural lipid and 5 mol% poly(ethylene glycol) (PEG) containing synthetic lipid. However, the steric constrains of large-sized PEG and the force exert by these polymers to the membrane destabilizes the resulting liposome, which necessitates the stabilization by cholesterol. Therefore, a roughly equimolar ratio of natural phospholipid and cholesterol is required. While cholesterol stabilizes the liposome membrane, it also reduces its flexibility and lateral mobility – two physical properties that are essential for biomimicry.[1] This is the reason why new strategies are needed to generate monocomponent synthetic cell membranes with stealth properties while maintaining a biomimetic system.

Amphiphilic Janus dendrimers (JDs) are known to self-assemble into dendrimersomes (DSs) which amalgamate many biomimetic physical properties such as a bilayer thickness of ~ 5 nm, high flexibility, mechanical stability and lateral mobility.[2] Due to their modular synthesis, their physical properties and their interactions with the environment can be tuned by rational design. We synthesized JDs that incorporate PEG or zwitterionic moieties, known to prevent protein and cell adsorption onto surfaces, in their hydrophilic section.[3]

With DSs self-assembled from these JDs, we aim to study selective interactions between specific ligands and receptors in the future.

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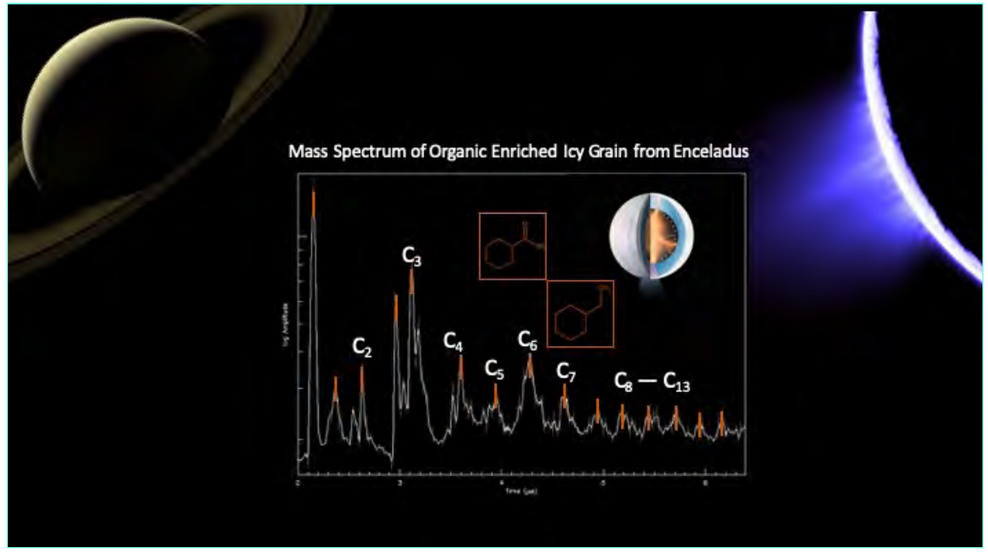

EXPLORING THE BIOGEOCHEMISTRY OF EXTRATERRESTRIAL ACTIVE OCEAN WORLDS

Nozair Khawaja, **Fabian Klenner, Jon Hillier, Frank Postberg, Marie Dannenmann, Zenghui Zou**
Inst. of Geological Sciences, Freie University Berlin, Germany

Saturn's moon Enceladus (and potentially Jupiter's moon Europa) has a subsurface liquid water ocean that interacts with its rocky core via hydrothermal vents. From its ocean, Enceladus emits a plume of gas and ice grains into space through fractures near its south pole. This plume was sampled by mass spectrometers on the Cassini spacecraft — the Cosmic Dust Analyzer (CDA) and the Ion and Neutral Mass Spectrometer (INMS). Alkaline hydrothermal vents on Enceladus, likely to be similar to those believed to be possible sites for the emergence of life in Earth's oceans, were confirmed by INMS and CDA detections of H_2, CH_4[1] and nanometre-sized silica particles[2]. Additional discoveries of biologically-relevant N-, O- and aromatic low- and high-mass organic compounds[3,4] reveal complex and reactive organic chemistry within the moon. We use Laser-Induced Liquid Beam Ion Desorption (LILBID) time of flight mass spectrometry, a proven analogue for CDA in situ ice grain mass spectrometry, to infer the biogeochemistry of Enceladus' ocean by comparing the LILBID mass spectra of selected compounds with those from CDA. Geochemically-relevant salts, as well as biologically-relevant organics, such as amino acids, fatty acids and peptides[5a], have been tested, and identified in the resulting mass spectra. Biotic and abiotic mass spectral fingerprints could be discriminated and biomolecule detection limits were found to be at the µM to nM level[5b], while those for salts (including sulfates and phosphates) are currently being measured and applied to CDA spectra. Further biological samples such as bacterial DNA and lysed cell material are under evaluation. The results we summarise here aid planning for future space missions to active ocean worlds.

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ULTRASTRUCTURAL ANALYSIS OF NUCLEAR PORE COMPLEX ASSEMBLY IN EARLY DROSOPHILA EMBRYOS BY CRYOFIB LIFTOUT

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[2] European Molecular Biology Laboratory, Structural and Computational Biology Unit, Heidelberg, Germany
[3] Max Planck Institute for Biophysics, Frankfurt am Main, Germany

For more than a century, Drosophila melanogaster has been one of the most prevalent model organisms in developmental biology. Recently discovered, D. melanogaster shows a non-canonical pathway of nuclear pore complex (NPC) biogenesis in early development that is likely present in other metazoans[1]. NPCs pre-assemble within so called annulate lamellae (AL) – sheets of endoplasmic reticulum – that insert into the nuclear envelope (NE) during early development to maintain a constant NPC/NE ratio. Due to the loss of ultrastructural information in classical plastic-embedded samples, the structural details of this process remain elusive. Structural analysis of multicellular organisms at cryo-temperatures by transmission electron microscopy has recently been made possible by cryo-focused ion beam milling and lift-out[2]. However, the procedure is tedious and time-consuming. Here, we present software and hardware solutions to improve the throughput and streamline the procedure for a reliable and robust workflow. With these developments, we are now able to study the ultrastructure of NPC assembly and AL insertion during early Drosophila development at unprecedented resolution. The membrane remodeling and protein condensation principles[3] that underlie this process have the potential to give ideas on the governing mechanisms in early eukaryotic life.

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FLOOR 6

EVOLUTIONARY OPTIMIZATION OF EXPERIMENTAL SYNTHETIC NETWORKS

Severin Angerpointner[1], Florian Gartner[1], Kai Kohler[2], Maren Haas[2], Erwin Frey[1], Oliver Trapp[2]
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[2] University of Munich (LMU), Butenandtstr. 7-13, 81377 Munich, Germany

Up to date, the formose reaction is the most plausible pathway in molecular evolution leading to the formation of sugar molecules. A plethora of monosaccharides is formed by dimerization of formaldehyde, subsequent (retro-)aldol reactions and aldose-ketose-isomerizations in the presence of basic catalysts.[1] Albeit Breslow had suggested an auticatalytic cycle starting as soon as traces of glycolaldehyde have been formed,[2] the initial dimerization of formaldehyde has not yet been mechanistically elucidated. In this collaboration project an extended formose reaction network will be comprehensively studied. The interplay of improved separation and analytic techniques with modern computer-aided simulations based on sloppy models[3] is the basis for tackling these challenges.

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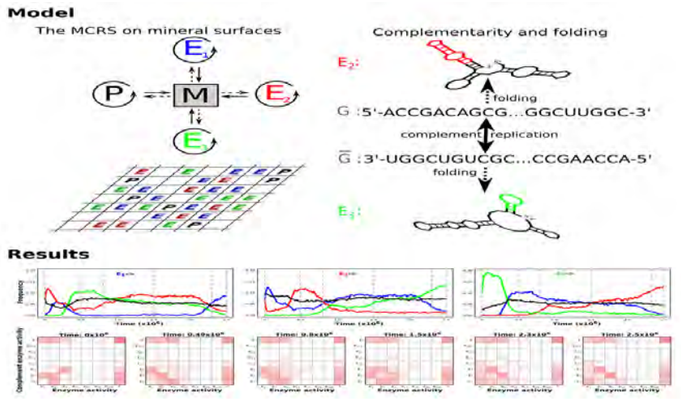

DYNAMICS AND STABILITY IN PREBIOTIC INFORMATION INTEGRATION: AN RNA WORLD MODEL FROM FIRST PRINCIPLES

András Szilágyi[1,2,3], Balázs Könnyű[1,4] & Tamás Czárán[1,2,5]

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[3] Center for Conceptual Foundation of Science, Parmenides Foundation, Kirchplatz 1, 82049, Pullach/Munich, Germany.
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The robust coevolution of catalytically active, metabolically cooperating prebiotic RNA replicators were investigated using an RNA World model of the origin of life based on physically and chemically plausible first principles. The Metabolically Coupled Replicator System assumes RNA replicators to supply metabolically essential catalytic activities indispensable to produce nucleotide monomers for their own template replication. Using external chemicals as the resource and the necessary ribozyme activities, Watson-Crick type replication produces complementary strands burdened by high-rate point mutations (insertions, deletions, substitutions). Metabolic ribozyme activities, replicabilities and decay rates are assigned to certain sequence and/or folding (thermodynamical) properties of single-stranded RNA molecules. Short and loosely folded sequences are given replication advantage, longer and tightly folded ones are better metabolic ribozymes and more resistant to hydrolytic decay. We show that the surface-bound MCRS evolves stable and metabolically functional communities of replicators of almost equal lengths, replicabilities and ribozyme activities. Being highly resistant to the invasion of parasitic (nonfunctional) replicators, it is also stable in the evolutionary sense. The template replication mechanism selects for catalytic "promiscuity": the two (complementary) strands of the same evolved replicator will often carry more than a single catalytically active motif, thus maximizing functionality in a minimum of genetic information.

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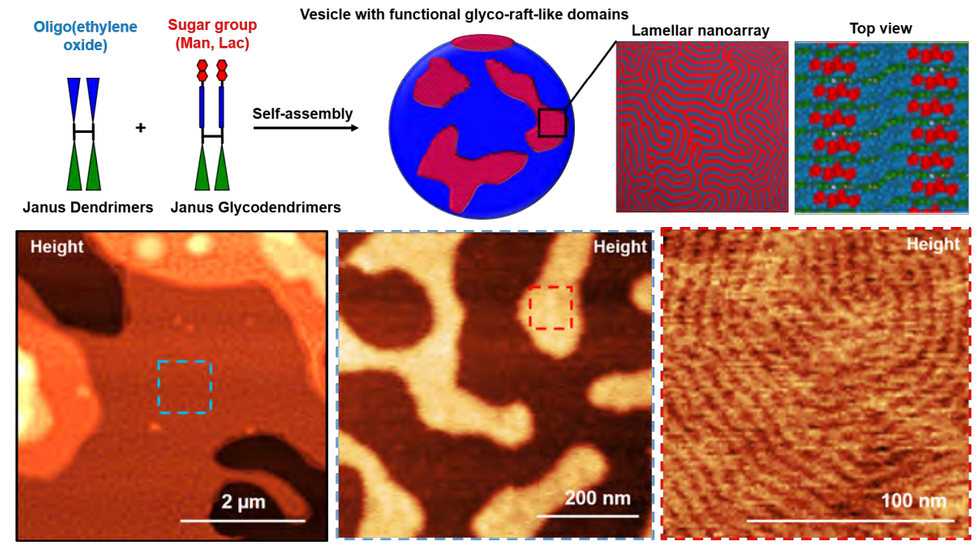

SUGAR-DRIVEN FORMATION OF ARTIFICIAL RAFT-DOMAINS WITH HIERARCHICAL PERIODIC NANOARRAYS ON DENDRIMERSOME PROTOCELLS

Nina Yu. Kostina[1], **Dominik Söder[1], Anna Wagner[1], Tamás Haraszti[1], Khosrow Rahimi[1], Virgil Percec[2], César Rodriguez-Emmenegger[1]**

[1] DWI- Leibniz Institute for Interactive Materials and Institute of Technical and Macromolecular Chemistry RWTH Aachen University, Forckenbeckstraße 50, 52074 Aachen, Germany
[2] Roy & Diana Vagelos Laboratories, Department of Chemistry, University of Pennsylvania Philadelphia, Pennsylvania 19104-6323, United States.

The seminal fluid mosaic model of the cell membranes suggests a lipid bilayer sea, in which cholesterol, proteins, glycoconjugates, and other components are swimming. Complementing this view, a microsegregated rafts model predicts clusters of components that function as relay stations for intracellular signaling and trafficking. Despite decades of work, the structure and function of these domains in cells remains difficult to resolve. Their immense complexity of functions arises from the combination of the chemical diversity of sugar moieties and their spatial 3D presentation. To tackle this challenge, we synthesized Janus dendrimers (JDs) and Janus glycodendrimers (JGDs) decorated with sugar moieties that in water self-assemble into vesicles that function as biological membrane mimics. We discovered that JGDs, on which the sugar groups were diluted in a defined way among tri(ethylene oxide) units, gave rise to lamellar or hexagonal nanoarrays and elicits higher bioactivity to sugar-binding proteins.[1,2] But could such nanoassemblies be preorganized into functional domains that mimic raft-domain in cells? And could the phase-separation be driven by solely hydrophilic interactions between amphiphilic molecules without the addition of cholesterol? We study the co-assembly of JDs (hydrophilic dendron decorated by tri(ethylene oxide)) with JGDs (decorated by sugar moieties). Our studies revealed that the sizes and nanoarrays of raft-like domains can be controlled by the ratio of JD to JGD and sugar type and that phase separation occurs only by hydrophilic interactions between tri(ethylene oxide) and sugar groups. The studies on understanding the formation of glycan periodic nanoarrays may help to shed light on cell communication and signaling and provide a powerful example in which structure determines function.

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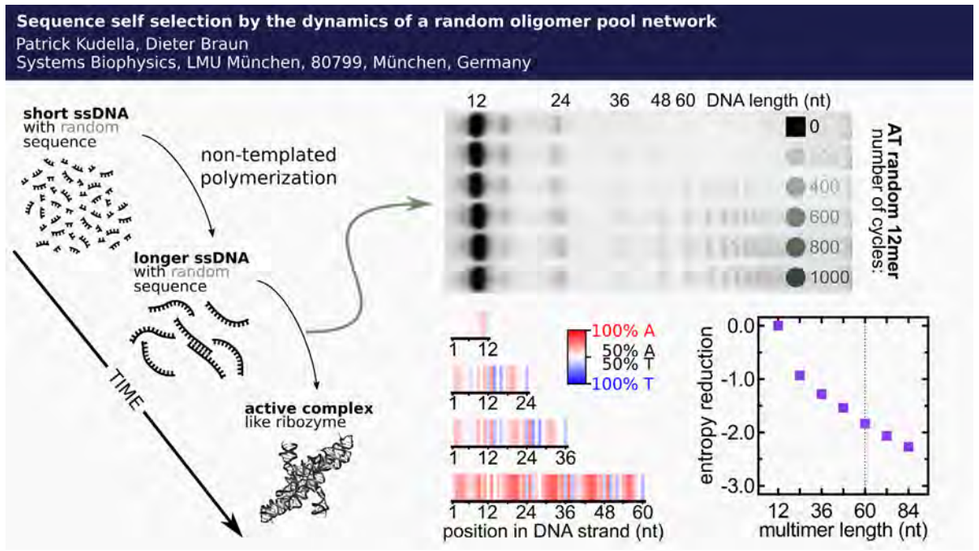

SEQUENCE SELF-SELECTION BY THE DYNAMICS OF A RANDOM OLIGOMER POOL NETWORK

Patrick Kudella, **Dieter Braun**
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Replication of information on oligonucleotides such as RNA or DNA is essential for the emergence of life[1,2]. Previous studies focus on the replication of single sequences, but we believe it is the key to monitor selection dynamics and replication starting in an already completely random pool of sequences. Theoretical work suggests a significant reduction in sequence entropy and therein a selection of a subset of the "fittest" sequences in a dawn of life scenario[3]. We expect a nonlinear ligation dynamic had set in, once polymerization was able to create oligomers long enough for hybridization and thus capable of structure formation and templated ligation. This "mechanism naturally involves the information transmission from a template to the newly ligated chain, thus opening an exciting possibility of long-term memory and evolvability"[3]. In the experiments we show how a system of 12mer random sequence DNA reduces its information entropy dramatically under an enzyme based template ligation reaction and temperature cycling. We obtained more than 12 million individual strands by Next Generation Sequencing (NGS). Utilizing a selfwritten LabView code we can study different mechanisms such as the emergence of a position dependent sequence pattern and a segregation into mutually complementary pools of A-rich and T-rich sequences. Both effects are associated with the development of a multiscale ligation landscape with multiple mutually catalyzing subpopulations.

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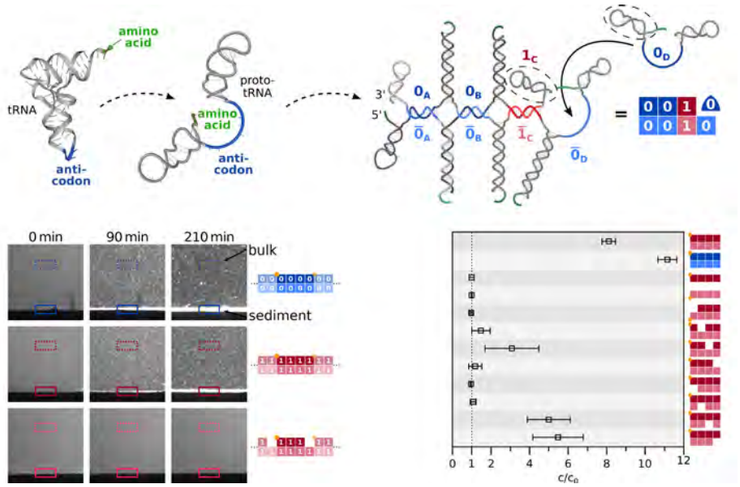

SEQUENCE DEPENDENT GELATION, ACCUMULATION AND SEDIMENTATION

Alexandra Kühnlein[1], **Thomas Matreux[1], Deni Szokoli[2], Hannes Mutschler[2], Dieter Braun[1], Christof B. Mast[1]**
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[2] Max Planck Institute of Biochemistry, Martinsried, Germany

The origins of biological information constitute a major challenge for understanding the origins of life. Under Darwinian evolution, a localized, homogeneous genotype is selected. A first attempt would be to start from a random sequence pool. The emerging state of matter converges towards a phenotype that is optimal under a given selection pressure, e.g. a physical non-equilibrium. To jumpstart Darwinian evolution, the random sequence pools must show physical phenotypes. The question is, however, how to obtain such a process without already evolved replicases in a naïve system.

Firstly, we show preliminary results that indicate a self-selection of sequences by cooperative binding. We started from a pool of eight complementary hairpins, inspired from tRNA, designed to build a hybridization based self-replicator[1]. To initialize the sample, we heat it up to 95°C to melt all prevailing hydrogen bonds. Upon subsequent cooling, we observe sudden agglomeration of DNA in the system. These agglomerates sediment under gravity. If one of the eight sequences are missing, no significant gelation and no sedimentation occurs.

Secondly, we subject a pool of random sequences to thermal gradients, where convection and thermophoresis can lead to size-dependent accumulation.

Through analysis on native PAGE gels[2], Illumina-Sequencing and subsequent MFE calculations we analyse if and how the initially random sequence pools are biased by the temperature gradient. We speculate that in the long run, only a reduced number of cooperative binding sequences could remain in such a non-equilibrium setting.

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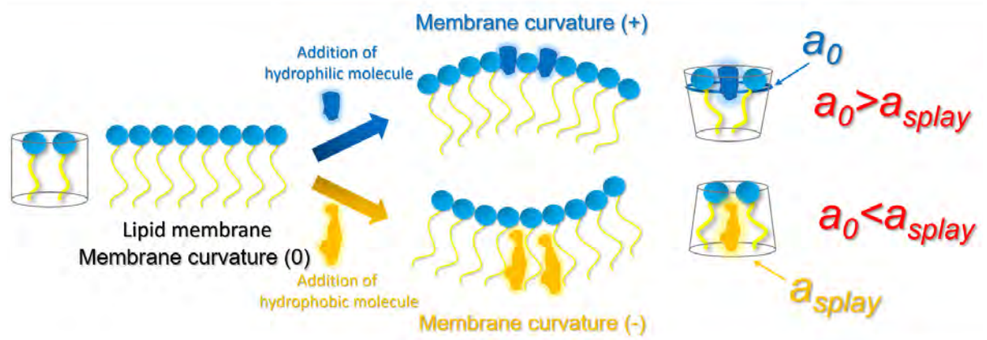

ESTIMATING PREFERENTIAL LOCALIZATION OF INTERACTING MOLECULES IN MODEL LIPID MEMBRANES

Chandrashekhar V Kulkarni
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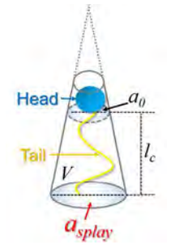
Spectroscopic techniques, in particular NMR, adequately reveal physicochemical interactions among a diverse set of molecules. However, when it comes to viscoelastic systems, including lipid phases, the applicability of these techniques remains limited due to poor signal quality caused by restricted diffusion. Here we present a novel method to estimate preferential localization of various molecules in lipid systems. This method is based on our recent work on 'chain splay'[1] and its relevance in quantifying molecular shapes of amphiphilic molecules, including lipids.

Figure 1: Commonly adopted truncated (inverse) conical shape by a majority of lipid molecules
By employing molecular level parameters (Figure 1), namely cross-sectional area at the head group (a0), lipid chain length (lc), molecular volume (V) and chain splay area (asplay) [1], one can perform quantitative estimation of an average shape of the amphiphilic molecule. Here, we show that by comparing above parameters with the parameters obtained after adding an additive molecule, it is possible to assess where that molecule prefers to localize within the membrane. This work finds great potential in formulating lipid systems for loading and interaction of a wide range of drugs and biomolecules exhibiting hydrophilic, hydrophobic or amphiphilic characters.



1 Kulkarni, C.V.* Calculating the 'Chain Splay' of Amphiphilic Molecules: Towards Quantifying the Molecular Shapes (2019) Chemistry and Physics of Lipids, 218, pp 16-21.

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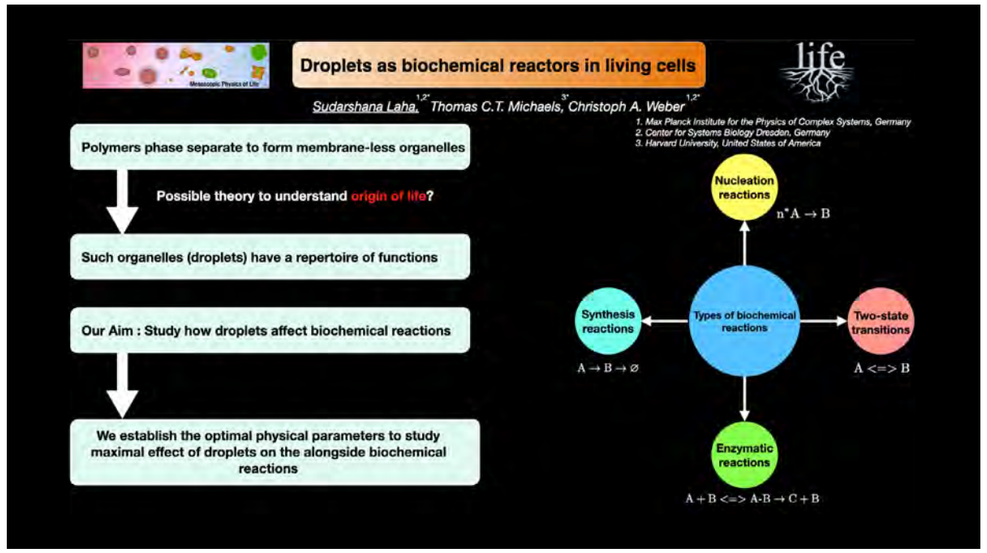

DROPLETS AS BIOCHEMICAL REACTORS IN LIVING CELLS

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[2] Center for Systems Biology Dresden, Germany
[3] Harvard University, United States of America

Living cells use compartments (droplets) to spatially organise molecules that can undergo fuel-driven chemi-cal reactions[1]. Not much is known about the mechanisms underlying such spatial control of chemical reactions and how much the properties of chemical reactions are altered by the compartments relative to homogenous systems. Here, we derive a theoretical framework to study fuel driven chemical reactions in the presence of compartments. We study two state transitions like phosphorylation via hydrolysis of ATP and enzymatic reactions. For two state transitions, we find that the ratio of phosphorylated product can be regula-ted by droplets by two orders of magnitude relative to the homogenous state. In the case of enzymatic reac-tions, we show that the initial rate of product formation can be increased by more than ten fold. We further calculate analytically the optimal conditions of designing the system. Our studies exemplify the enormous potential of phase separated compartments as biochemical reactors in living cells and enhancing the effect of enzymes.
Understanding the control of biochemical reactions via compartments is key to elucidate the func-tionality of stress granules for the cell and is also crucial for biochemical communication among synthetic cells and RNA catalysis in coacervate protocells.

1 Considerations and challenges in studying liquid-liquid phase separation and biomolecular condensates, Tanja Mittag et al., Cell, 2019

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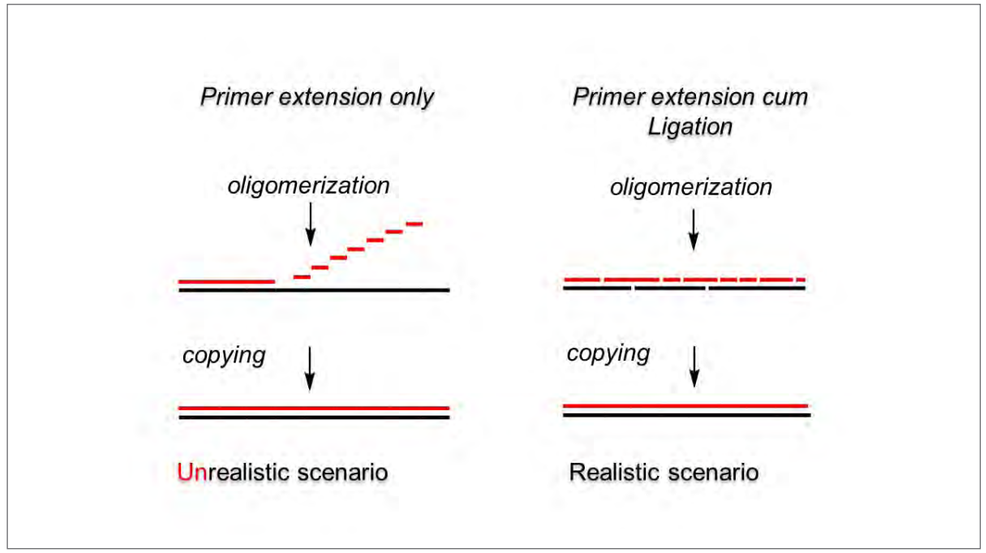

BRIDGING THE GAP BETWEEN CHAIN FORMATION & GENETIC COPYING OF RNA

Gabrielle Leveau[1], **Tobias Göppel[2], Daniel Pfeffer[1], Joachim Rosenberger[2], Ulrich Gerland[2], Clemens Richert[1]**
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The copying of RNA sequences is the template-directed reaction underlying replication. It is interesting to ask how such a process may have occurred in a prebiotic context to ensure the transmission of genetic information.
A minimal living system, from which more complex systems can arise via Darwinian evolution, must be able to replicate its genetic information. Steps toward such a minimal system should include the formation of oligonucleotide chains and their copying through the formation of complementary strands. Thus far, creating a minimal evolving system in the laboratory has remained elusive for RNA, and there are gaps in our understanding of this aspect of prebiotic evolution. One prominent gap is between the formation of short oligonucleotides from nucleotides and the spontaneous emergence of a copying process that can maintain and propagate the sequence information encoded in a minimal genome. Experiments in the absence of a polymerase show a sequence fidelity too low for inheriting even short genes. They are also not prebiotically plausible, given that they rely on one primer-template complex that is extended by monomers only, as in modern-day PCR reactions, and not a statistical mixture of different strand lengths expected for oligomerization products. Still, selective and efficient incorporation of activated monomers has been demonstrated, using immobilized template/primer systems.[1] We are expanding this work to enzyme-free ligation of dimers or trimers to an RNA primer using in situ activation conditions.[2] A quantitative modeling of RNA copying is also being conducted. The challenge to achieve replication of a short RNA sequence, a feat recently accomplished for 3′-amino-2′,3′-dideoynucleotides and an initial DNA template,[3] will be discussed.

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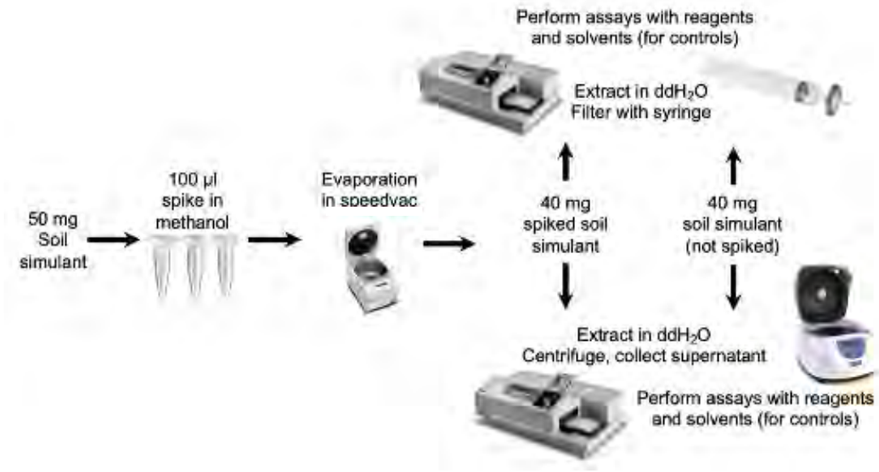

BIOCHEMICAL METHODS FOR THE DETECTION OF PROTEINS AS LIFE SIGNATURES ON MARS-LIKE SOILS

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One of the principal objectives for planetary exploration is the search for traces of past life and evidence of conditions that may have supported life. Such analytical approaches often rely on the detection of specific markers (i.e. biomolecular signatures) and require the development of highly specialised methods and complex automated analytical platforms. The high cost of such missions is matched by the high risk of failure (i.e. mechanical failure, crash landing, loss of vehicle during launch, loss of contact, instrument failures, etc). Development of simple, highly specific, and conclusive assays with a minimum number of steps would mitigate many of the risks and improve the efficacy of such explorative tests. Astrobiological research is also oriented in Mars-like soil samples on Earth which provide an analogue for experimental design and simulation. In this study, we present simple methods to quantify proteins on Martian soil simulants with a long-term goal the development of a fully automated platform for future exploration missions.

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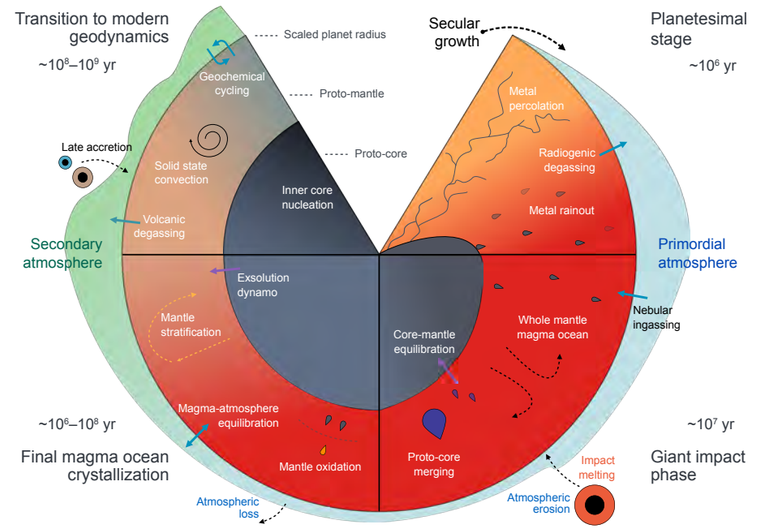

ATMOSPHERIC SPECIATION OF ROCKY PLANETS FROM MAGMA OCEAN OUTGASSING

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[4] Institute of Geochemistry and Petrology, ETH Zurich

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The earliest atmospheres of rocky planets originate from extensive volatile release during one or more magma ocean epochs that occur during primary and late-stage assembly of the planet[1]. These epochs represent the most extreme cycling of volatiles between the interior and atmosphere in the history of a planet, and establish the initial distribution of the major volatile elements (C, H, N, O, S) between different chemical reservoirs that subsequently evolve via geological cycles[2].

Crucially, the erosion or recycling of primary atmospheres bear upon the nature of the long-lived secondary atmospheres that will be probed with current and future observing facilities[3]. Furthermore, the chemical speciation of the atmosphere arising from magma ocean processes can potentially be probed with present-day observations of tidally-locked rocky super-Earths[4]. The speciation in turn strongly influences the climatic history of rocky planets, for instance the occurrence rate of planets that are locked in long-term runaway greenhouse states[5].

We will present an integrated framework to model the build-up of the earliest atmospheres from magma ocean outgassing using a coupled model of mantle dynamics and atmospheric evolution. We consider the diversity of atmospheres that can arise for a range of initial planetary bulk compositions, and show how even small variations in volatile abundances can result in dramatically different atmospheric compositions. We will discuss our results in light of the prospects for untangling the diversity of rocky planetary atmospheric compositions and their potential effects on the redox state of the earliest mantle geochemistry and atmospheric speciation relevant for surficial prebiotic chemical environments[6,7].

Only through the lense of coupled evolutionary models of terrestrial interiors and atmospheres can we begin to deconvolve the imprint of formation from that of evolution, with consequences for how we interpret the diversity revealed by astrophysical observables, and their relation to the earliest planetary conditions of our home world.

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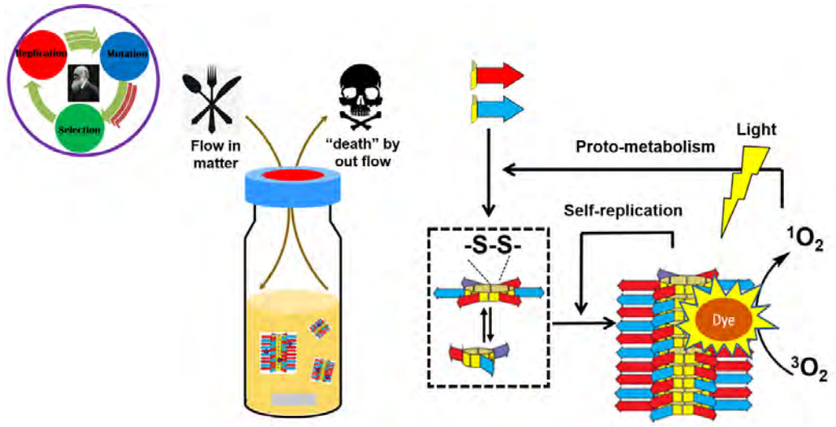

TOWARDS DARWINIAN EVOLUTION OF SYNTHETIC REPLICATORS

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NASA's working definition for life is "a self-sustaining chemical system capable of Darwinian evolution"[1]. In biology, Darwinian evolution can be considered to be the result of an interplay of replication, mutation, and selection[2]. These concepts can be extended to chemical systems. Otto group has realized exponential self-replication through elongation/breakage of a fibre[3]. Starting from two different building blocks, diversification of replicators is achieved through cross-catalysis[4]. Recently we find replicator can recruit and activate a photocatalytic cofactor, catalysing the synthesis of its own precursors to promote replication[5]. The photocatalysis is presumed to work as "encoded function" that may be selected in a replication-deconstruction regime. When mutant replicators with different catalytic ability are subjected to flow condition, most photoactive ones become dominant, reminiscent of "survival of the fittest".

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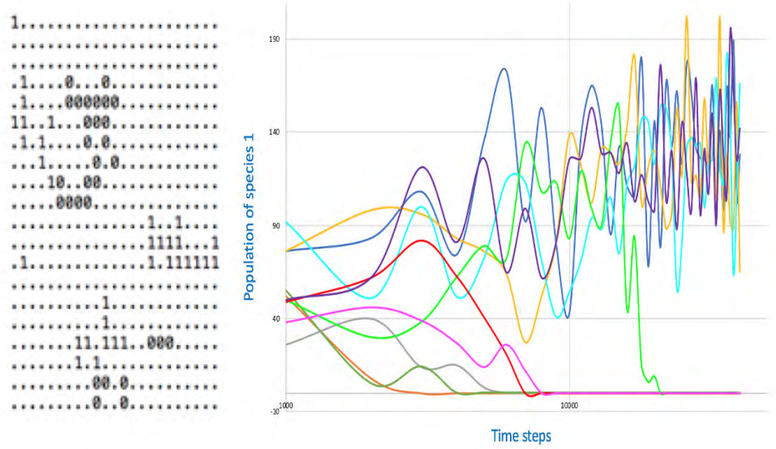

ANOMALOUS FLUCTUATIONS AND SELECTIVE EXTINCTION IN PRIMORDIAL REPLICATORS: A "STRUGGLE FOR LIFE" AT THE ORIGIN OF BIOLOGICAL CHIRALITY

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The prevalent presence of a single chiral variant of molecules in live organisms is one of the most distinctive signs of life as a global phenomenon. One of the greatest ambitions of Biochemistry and Astrobiology is to provide an explanation of this predominance. Several mechanisms were proposed in the past, based on the "propagation" of chirality from a homo-chiral substrate and the amplification of effects associated with electro-weak interaction. Here, a different scenario is proposed: anomalous fluctuations associated with a self-replication scenario can lead to selective extinction of one of the two variants[1]. These fluctuations arise spontaneously when a global (not a local one) feedback acts. The idea is based on two key-points: a) the simulation of prebiotic processes as a "chessboard play"[2]; b) the presence of great fluctuations during an autocatalytic process[3]. In order to demonstrate this mechanism, a computational model is developed, describing the "struggle for life" of two different kinds of primordial replicators in a n×m chessboard, with a periodic contour; each replicator employs catalyzers of different chirality but on a non-chiral substrate, thereby with no selective advantage. The replication occurs randomly and with a fixed probability, providing that a sufficient amount of chemical energy is locally available. Results clearly show that strong fluctuations in the number of individuals of each species and a subsequent selective extinction of one of the two are observed. These studies may contribute to shed light on a most mysterious phase transition occurred during the biochemical evolution of our planet.

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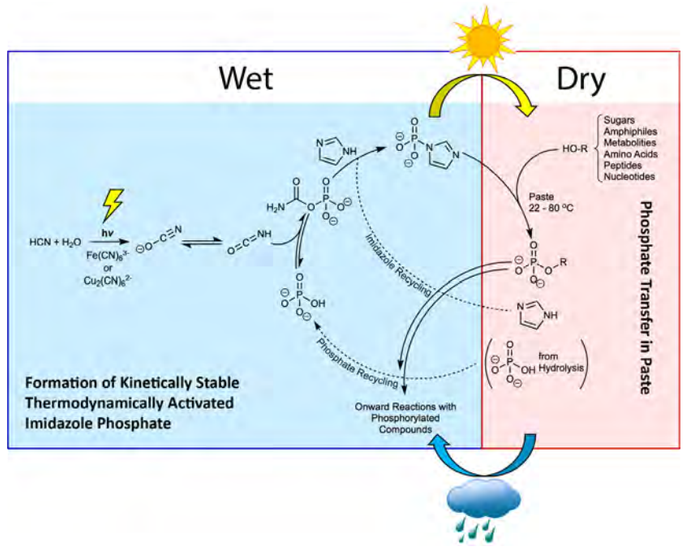

CYCLING OF ORTHOPHOSPHATE UNDER MILD PREBIOTICALLY PLAUSIBLE CONDITIONS

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Phosphate-based chemistry is crucial to Life and extant Life is able to continuously activate, transfer and recycle orthophosphate in order to drive cellular biochemistry. However, in prebiotic chemistry the activation of orthophosphate from geochemical sources and subsequent transfer to prebiotically important organic compounds under mild conditions remains an outstanding fundamental challenge. Considering the paucity of prebiotically plausible phosphorylating reagents and reaction conditions that can directly activate and transfer phosphate in a single reaction step, we sought an alternative primordial scenario whereby the phosphate activation step and phosphate transfer step are separated. Conversion of an activated form of phosphate into a kinetically stable thermodynamically activated molecule would enable the accumulation of an activated form of phosphate in solution. Subsequent drying down of the solution into a paste could then enables the transfer of the phosphate.

Here, we demonstrate that we can use isocyanate to activate orthophosphate and store the energy in the phosphoramidate imidazole phosphate. Initiation of a wet/dry cycle enables transfer of phosphate to a diverse range of prebiotically important organic compounds. Upon re-wetting, orthophosphate can be reactivated, and the cycle repeated. This approach enables orthophosphate to be continuously recycled and converted back into an activated form under mild conditions thus establishing a prebiotic analogue of the system by which extant Life cycles orthophosphate.

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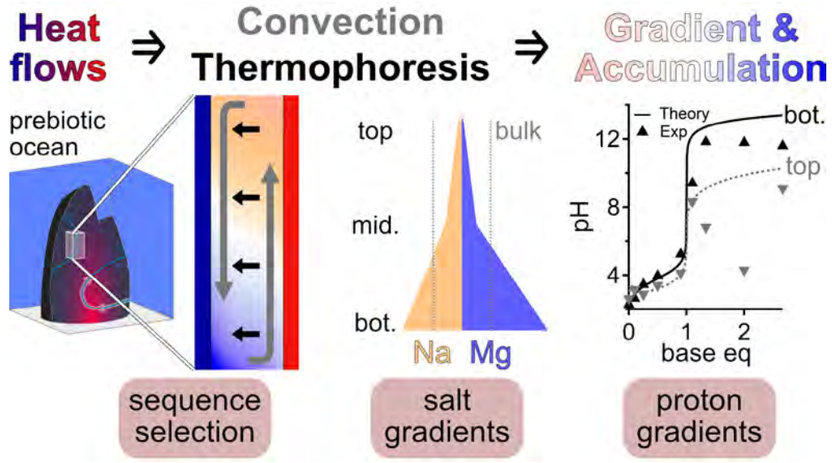

HEAT FLOWS SHIFT CHEMICAL EQUILIBRIA BY SELECTIVE ACCUMULATION

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

The reaction chambers are sandwiched between highly heat conducting sapphire plates ensuring complete thermal control including possible thermal gradients. Microfluidic structures are made from FEP, which lets us focus on the interactions between the molecules. Ions leached from prebiotically plausible mineral samples are selectively accumulated by thermal gradients and permit enzymatic activity. Thermal non-equilibrium boundary conditions drive concentration gradients, enabling chemical reactions and generating and controlling pH gradients in a plausible prebiotic scenario. Local gradients driven by heat fluxes will offer unique opportunities to enable molecular selection and evolution at the origins of life.

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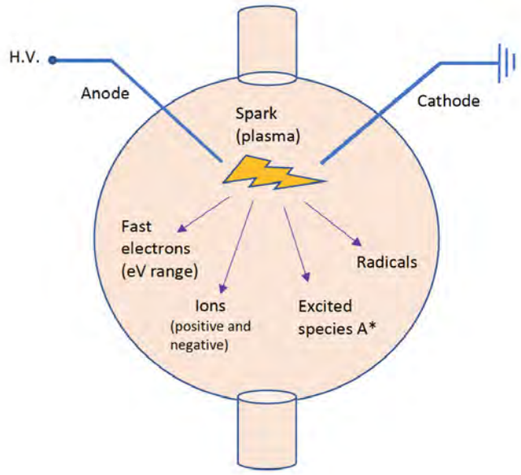

NEW INSIGHTS ON PREBIOTIC CHEMISTRY FROM PLASMA KINETICS

Gaia Micca Longo[1,2], **Vincenzo Laporta[2], Savino Longo[1,2]**
[1] Department of Chemistry – Università degli Studi di Bari Aldo Moro – Via Orabona 4 – 70125 Bari, Italy
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The famous Miller-Urey experiment[1], which provides essential insight on the prebiotic synthesis of the molecules of life, still has many obscure points. Although the theoretical studies on Miller's experiment are very advanced[2], one aspect of these studies is still rather primitive, namely the role of electrons in the plasma in producing the first excited and radical species and ions, which later enter several chemical channels to form prebiotic molecules. Here, we want to suggest a way of possible future progress: framing the experience of Miller and Urey in the context of the kinetics of ionized gas, or plasma. In this context, effective and versatile theoretical tools, based on quantum mechanics and chemical kinetics, make it possible to look, in a new way, at the elementary processes that lead to the formation of excited species and ions, at the origin of the cascade of subsequent reactions.
Two new elements may produce a synergistic push towards further progresses: a) the awareness that the primordial atmosphere was not at all the strongly reducing mixture believed in Miller's times; b) the development of new methods in the context of computer modeling of the kinetics of plasmas. The communication between the two communities of plasma kinetics and astrobiology can therefore help, in the future, to attain a better understanding and new insights on the chemical kinetics of an historical experiment, which has changed our ideas on the genesis of prebiotic molecules on the primordial Earth.

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Aligns with meeting schedule

THE FIRST STEP FROM MOLECULES TO LIFE: FORMATION OF LARGE RANDOM MOLECULES ACTING AS MICRO-ENVIRONMENTS

Saibal Mitra

The processes that led to life had to circumvent the limit on the complexity of low fidelity replicating systems[1]. I have proposed a three step process to address thus problem[2]. The first step takes place in a space environment where in ice grains large random molecules form under the influence of UV radiation and cosmic radiation. The structure of these molecules are those of 3 dimensional percolation clusters which are known to have a fractal structure[3,4]. Such molecules of a typical size of 100 nm have a porous structure that are permeable to small molecules.

The second step involves the formation of loosely bound aggregates of such random molecules on proto-planets in the early solar system. The third step involves biochemical processes taking place inside these aggregates. One can then consider conventional models of the origin of life inside the micro-environment within such aggregates instead of the raw outside environment. The fidelity problem is then addressed by the effective compartmentalization and fixed surface structures having a large effect on the biochemical due to the small size and the fractal structure of the environment.

The loosely bound aggregate will gradually erode, which will cause the micro-environment to gradually resemble the outside environment, providing for a mechanism for the biochemical system to gradually adapt to the outside environment.

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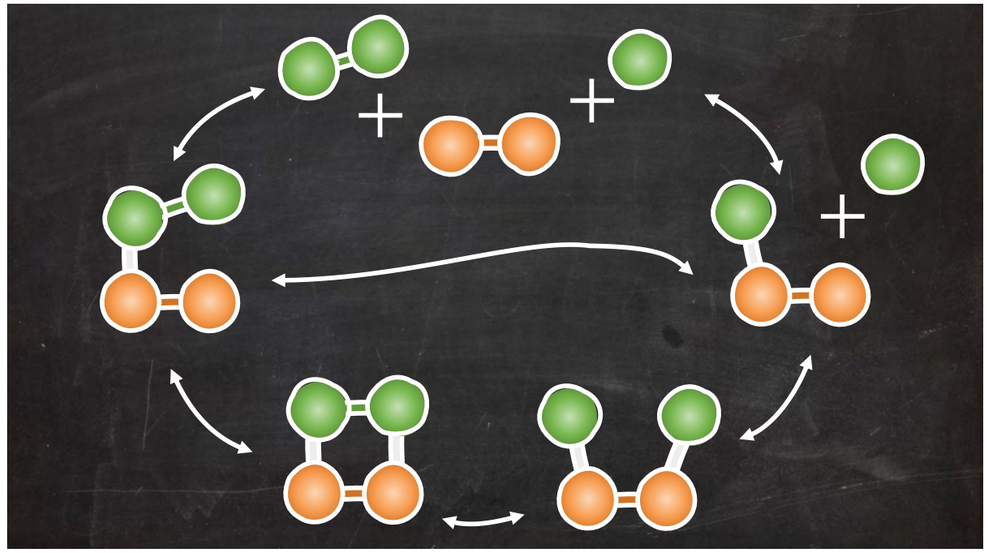

PHYSICS AND EVOLUTION OF CATALYST

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Enzymes are the unsurpassed catalysts of Nature, operating under mild conditions to produce reaction rate enhancements of several orders of magnitude[1]. Their remarkable catalytic activity is attributed to the high complementarity between the enzyme's active site and the transition state of the catalyzed reaction, a feature that has inspired the design of artificial enzymes and transition state analogs[2]. Despite outstanding progress in the field, the driving forces underlying catalysis still remain unclear[3]. Advances in singlemolecule enzymology provide unprecedented information of enzyme dynamics and catalytic mechanisms[4,5], making it timely to analyze the design principles and fundamental constraints of catalysts.

In our work, we search for the geometrical and physical constraints necessary for the emergence of catalytic activity in a system of DNAcoated colloids. We use coarse-grained computer simulations to build structures of increasing complexity with spherical colloids. Our goal is to identify the simplest structure with the potential to catalytically cleave a bond. 2D simulations show that a rigid dimer structure can provide a bond-breaking mechanism by binding strongly to the substrate and forming a rhomboidal configuration. We explore the optimal trade-off between strong binding and product release achieved in catalysts[3].

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PREBIOTIC CHEMICAL ENERGY FLUX

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Life on planet Earth may have started at sites of volcanic activity like deep sea hydrothermal vents, feeding on chemical energy of ejected matter in disequilibrium.[1,2] The project presented here explores flux of chemical energy under modelled primordial conditions which may have laid the foundation for biological energy metabolism prior to cellular life. In particular, we study energetic ramifications of the NiS-catalyzed carbonylation of thiomethanol yielding acetic acid, a possible pre-biotic carbon fixation reaction.[2] It is hypothesized that energy-rich intermediates (acetyl nickel species, methylthioacetate and possibly others) are evolutionary precursors of analogous intermediates in still prevailing metabolic pathways.[3,4] The poster illustrates experiments to determine formation and hydrolysis rates of key intermediates that are likely candidates for having served as gateways to the "thioester world"[4] and/or the establishment of a versatile biological "energy currency" like ATP or evolutionary precursors thereof.

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FLOOR 8

ON THE ORIGINS OF THE PROTEIN WORLD: A LARGE -SCALE COMPUTATIONAL APPROACH TO STUDY THE EMERGENCE OF THE FIRST AUTONOMOUSLY FOLDING PROTEINS

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Since the time of the Last Universal Common Ancestor (LUCA), proteins have been the fundamental catalysts of life. For their activity they must assume three-dimensional structures by a complex, easily disrupted, process of folding. However, it is still unclear how the first folded proteins emerged and how life came to rely so extensively on their ability to fold. Our hypothesis is that the first folded proteins resulted from the increased complexity of peptides in the "RNA-peptide world" that preceded LUCA, possibly by three mechanisms[1,2]: repetition, accretion, and recombination. While repetition is one of the most common mecha-nisms for the emergence of new folded proteins[3], and accretion could already be traced to a few ancient folds[4], recombination is a mechanism harder to trace.
Instead of searching for examples of folds that could have their origins in the recombination of at least two ancient fragments, we followed a large-scale computational approach to study whether two such fragments could generate a folded protein when recombined and excluded from their original scaffolds. Using the ribosome as a model of the primordial "RNA-peptide world"[1], we collected a set of ribosomal peptide fragments, which are only folded in the context of the ribosome, and followed an all-against-all molecular docking approach to evaluate their propensity to establish geometrically and energetically compatible inter-faces that would allow the formation of stable, globular, recombinant folds in the absence of the RNA. As a result, we identified multiple ribosomal peptide frag-ment pairs that can recreate not only frequent protein folds but also novel fold topologies and further optimised some of these folds by exploring the sequences of their parent fragments in different organisms. From these, we selected two pairs that are now being experimentally characterised, opening a door to a better understanding of the emergence of the first autonomously folding proteins.

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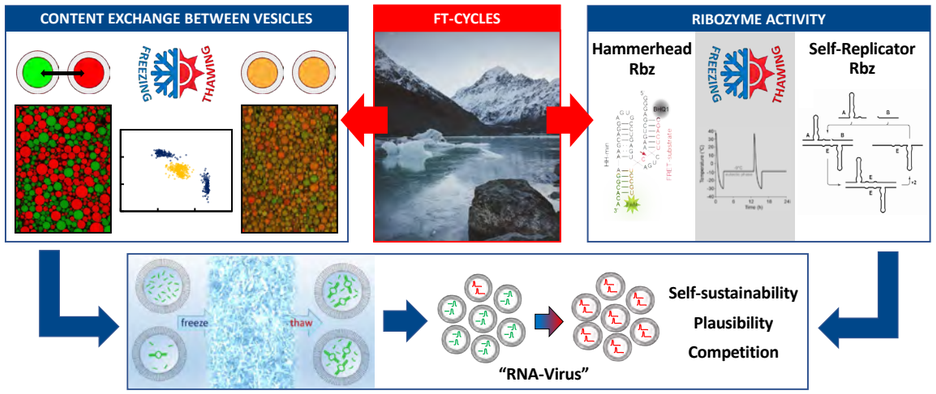

FREEZE-THAW DRIVEN PROLIFERATION OF RNA PROTOCELLS

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With the advent of compartmentalization in the RNA world, how were early protocells able to grow and proliferate without the sophisticated protein machineries found in modern forms of life? Based on previous studies of genetic exchange between giant unilamellar vesicles (GUVs), we seek to apply repeated freeze-thaw (FT) cycles as a physicochemical driver for the expansion of encapsulated self-replicating ssRNA enzymes (ribozymes). This system will serve as a model for the growth and proliferation of RNA protocells in the plausible geochemical environment of early Earth exhibiting diurnal freezing of water to ice.

Litschel T, Ganzinger KA, Movinkel Torgeir, Heymann M, Robinson T, Mutschler H, Schwille P (2018) New J Phys 20:055008
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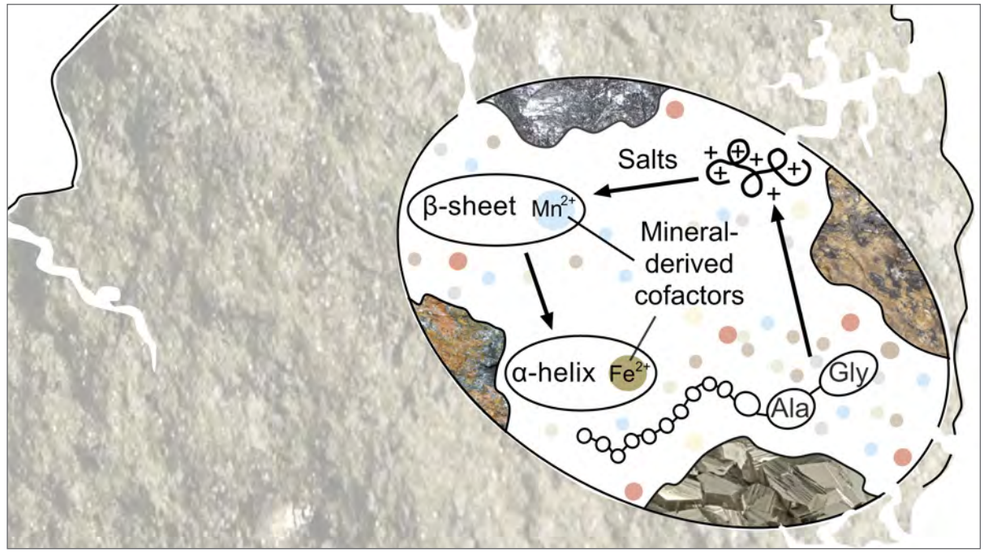

THE AMBIVALENT ROLE OF WATER AT THE ORIGINS OF LIFE

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Without water as a solvent and reactant, life as we know it would not exist. However, water molecules can also counteract the formation of essential organic molecules due to hydrolysis. This conundrum constitutes one of the central issues in origin of life research[1]. Hydrolysis is an important part of energy metabolism but only because inside a cell, it is a controlled reaction. How could hydrolysis have been regulated under prebiotic settings? Lower water activities possibly provide an answer. Geochemical sites with less free and more bound water can supply the necessary conditions for protometabolic reactions. Such conditions occur in serpentinizing systems, hydrothermal sites that synthesise hydrogen gas via rock–water interactions[2,3]. We summarise the parallels between biotic and abiotic means of controlling hydrolysis in order to narrow the gap between biochemical and geochemical reactions[4], and outline how hydrolysis could even have played a constructive role at the origin of molecular self-organisation[5].

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AMPHIPHILIC COMB-POLYMERS SOLVE THE DILEMMA OF POLYMER-BASED CELL-MIMETIC MEMBRANES

Khosrow Rahimi, **Mehrnoush Rahimzadeh, Jan Tenbusch, Nina Kostina, Cesar Rodriguez-Emmenegger**
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Natural membranes achieve an incredibly rich functionality by the self-assembly of different components at an almost invariable thickness (5±1 nm). Remarkably, in spite of their minute thickness and flexibility, natural membranes are incredibly stable. The combination of these seemingly antagonistic properties makes membranes a key for life to exist. The thickness and flexibility has been mimic by assembly of lipids into synthetic vesicles call liposomes. Nonetheless, liposome lack stability to environmental conditions, severely limiting their use for advance functions. Polymersomes from amphiphilic block copolymers display a much enhanced mechanical stability, but at the expense of thickness well above the natural ones and an almost complete stall of the dynamics compared to biological membranes. Furthermore, the mismatch between the membrane thickness and the size of transmembrane proteins has been the main obstacle hampering the integration of natural bioreceptors in polymersomes. Here, I present our advances in cell mimetic membranes based on amphiphilic comb polymer. The polymers consist of a hydrophilic highly flexible backbone to which fatty-acid-like side groups are appended. The latter drive the zipping of the polymer chains into bilayers. We developed an accelerated iterative combinatorial synthesis to generate a library with systematic structural variation. This allowed us to elucidate how to program the thickness, stability and flexibility in the molecular structure and topology of the polymer and in this way solve the dilemma of combine stability with extreme flexibility and biomimetic thickness. Contrary to block copolymer, no entanglement of hydrophobic domains occurs, thus the thickness and flexibility of our membrane mimic closely matches those of their natural counterparts. This is demonstrated by structural analysis of vesicles as well as by the insertion of transmembrane proteins. Our model hold promise for the design of interactive protocells.

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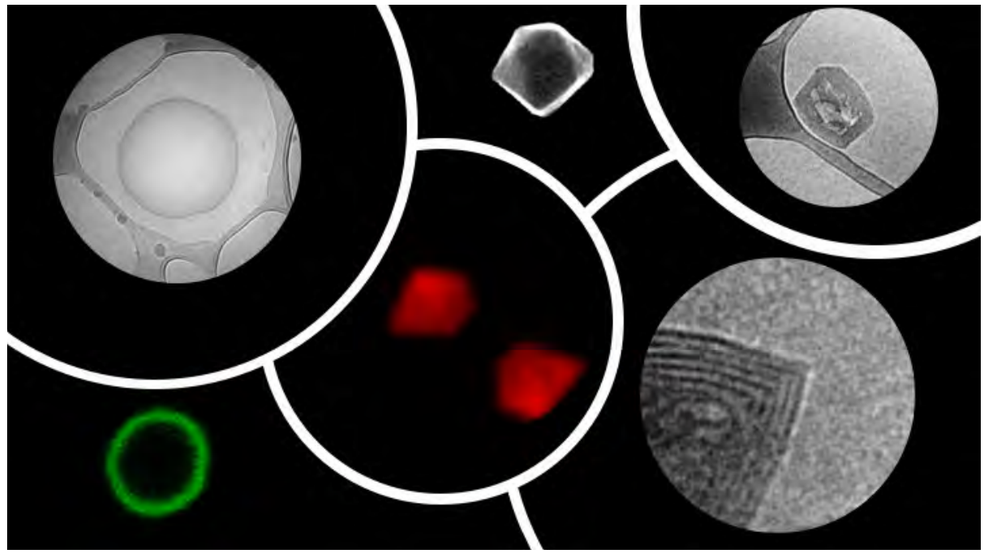

STRUCTURAL DESIGN OF AMPHIPHILIC COMB POLYMERS TO SELF-ASSEMBLE INTO FACETED MEMBRANE PROTOCELLS

Mehrnoush Rahimzadeh, **Jan Tenbusch, Khosrow Rahimi, Nina Kostina, Cesar Rodriguez-Emmenegger**
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Compartmentalization by self-assembly of lipids into membrane is a key element to the origin of life. Various synthetic and hybrid mimics have been developed based on the self-assembly of lipids or amphiphilic block copolymers aiming at recapitulating some properties of spherical membranes. However, other more complex morphologies are also present in nature. Particularly interesting are faceted membranes, in which the Gaussian and mean curvature of the membrane are zero like in Haloquadratum archaea, where cells are perfectly prismatic. Recapitulating such membranes requires a fine balance between surface energy, conformational entropy, and order, as the formation of sharp edges is extremely unfavorable in soft matter. To mimic this morphology, we developed a new family of amphiphilic comb-copolymers consisting of a poly(N-vinylacetamide) hydrophilic backbone to which we grafted hydrophobic side alkyl chains. However, to achieve faceted vesicle it is necessary to device a two-step self-assembly procedure. At temperatures above crystallization temperature of the side chains, the segregation between the backbone and side chains drives the assembly into bilayers of biomimetic thickness. By cooling the sample, the crystallization of side chains under the confinements of the membrane, forces a shape transformation from the spherical into polyhedral vesicles. The thermodynamic conditions for this transition are encoded in the side groups. Polymers with long alkyl chains (≥C18) in their extended and frozen state crystallize inside the bilayers in a planar hexagonal lattice. Since this packing is incompatible with spherical shape, it results in topological defects of various folds forming multiple facets. Indeed, comb polymers with low degree of substitution form faceted vesicles if the crystallization forces are strong enough (e.g. for C20). Our system hold promises to further elucidate the mechanisms behind the formation of complex living membranes in nature.

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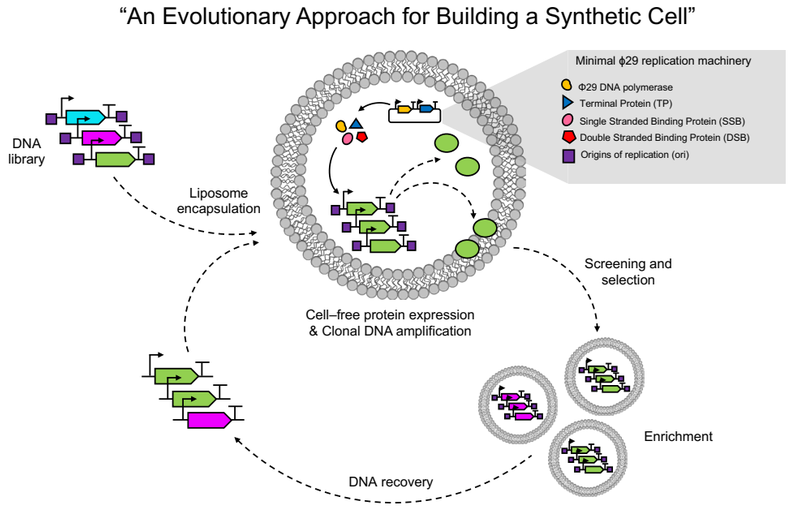

AN EVOLUTIONARY APPROACH FOR BUILDING A SYNTHETIC CELL

Ana M. Restrepo, **Zhanar Abil, Christophe Danelon**
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The goal of bottom-up synthetic biology culminates in the construction and engineering of a 'living' artificial cell. This grand challenge can be broken down into the reconstitution of essential cellular functions into an enclosing membrane, such that autonomous life-like properties as growth or division, will emerge. We propose to complement traditional strategies with an in vitro directed evolution approach, as an optimization scheme to implement the different fundamental biological modules. Specifically, in-liposome cell-free gene expression coupled with isothermal DNA amplification forms the basic unit for our evolutionary experiments. The PURE system is used as a minimal transcription-translation apparatus, while protein-primed DNA replication is performed by the Phi29 machinery. We established conditions for driving the function of the encoded protein when coupled to orthogonal DNA replication. Cases of study include auto fluorescent proteins, phospholipid-synthesizing enzymes and Phi29 replication proteins. We believe that when combined with the compartmentalized expression of a gene library, our directed evolution approach will accelerate the engineering of complex biological functions and, ultimately, of a synthetic cell.

Van Nies, P. et al. Self-replication of DNA by its encoded proteins in liposome-based synthetic cells. Nat Commun 9, (2018).

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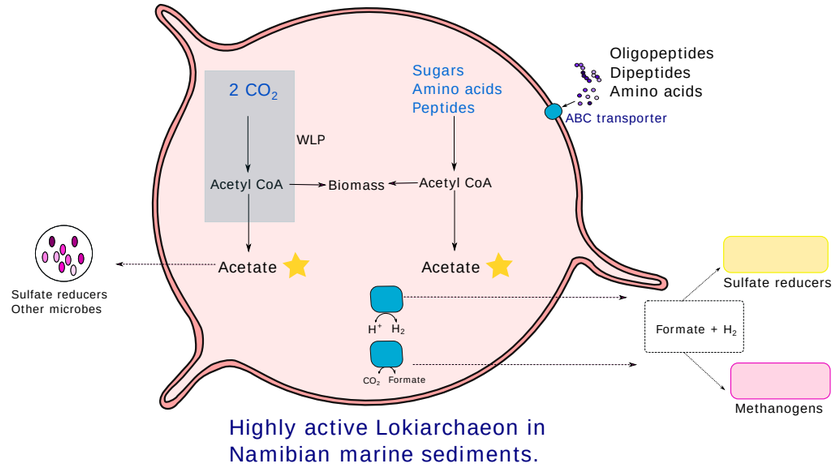

Highly active Lokiarchaeon in Namibian marine sediments.

LINKING MICROBIAL DIVERSITY TO CARBON CYCLING IN SUBSEAFLOOR SEDIMENTS FROM THE NAMIBIAN CONTINENTAL SHELF

Paula Rodríguez[1], **Ömer K. Coskun[2], Aurèle Vuillemin[2], William D. Orsi[2,3]**
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The Benguela Upwelling System (BUS) is one of the most productive ecosystems in the world (0.37 Gt carbon/year). This oceanographic feature exhibits a wind-driven, seasonal primary production that peaks during the austral winter when cold, nutrient-rich waters are injected into the photic zone. The increased primary productivity leads to a high export rate of organic carbon to the marine seafloor, where remineralization occurs, mainly driven by microbial metabolic processes such as sulfate reduction, denitrification, methanogenesis, methanotrophy and fermentation. Thus, carbon turnover in Namibian marine sediments plays a key role in large-scale nutrient losses and gains, oceanic N:P ratio dynamics and production of greenhouse gases such as CH_4, N_2O and H_2S. Here, a novel experimental approach known as quantitative Stable Isotope Probing (qSIP) was used to quantify ^{13}C incorporation into bacterial and archaeal 16S rDNA from subseafloor sediments of the Namibian Continental Shelf. Incubations from 28 cm depth carbonate-rich, sulfidic sediments were set up for ten days under anoxic conditions with [^{13}C] labeled bicarbonate and [^{13}C] labeled diatomaceous extracellular polymeric substances (dEPS). Experimental data shows DIC assimilation by a total of 1676 microbial operational taxonomic units (OTUs) primarily affiliated to Gamma and Deltaproteobacteria, Chloroflexi, Planctomycetes, Latescibacteria and Acidobacteria. Archaeal OTUs belonging to Bathyarchaeota, Euryarchaeota and Asgardaeota accounted for 52% of the [^{13}C] bicarbonate labeled populations. Lower levels for [^{13}C] dESP incorporation were measured, with a total of 329 enriched microbial OTUs mainly from the same taxonomic groups found enriched in the autotrophic incubation, likely indicating a bias towards consumption and cycling of organic matter produced in dark carbon fixation. This study gives insights into the ecological features of several uncultured groups and their metabolic activity. Furthermore, it sheds light on the taxonomic identity of key microbial populations performing biochemical processes linked to carbon turnover in Namibian Continental Shelf anoxic sediments.

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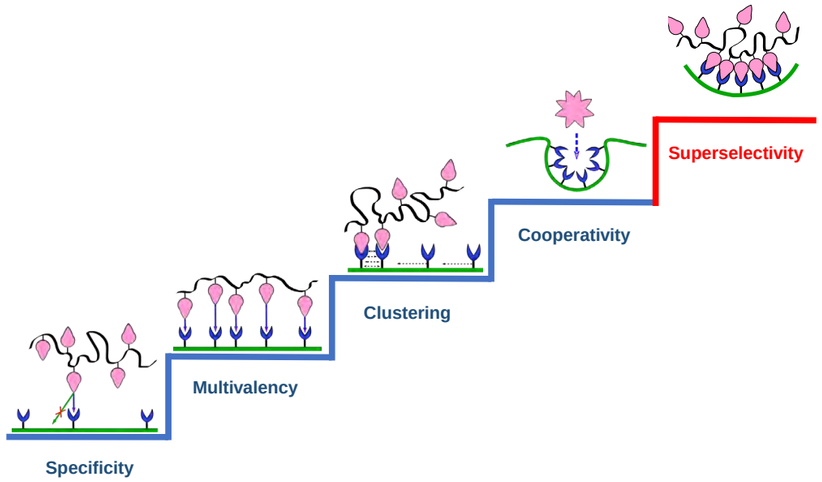

SUPERSELECTIVITY IN SYNTHETIC PROTOCELLS

Cesar Rodriguez-Emmenegger
DWI — Leibniz Institute for Interactive Materials.

I address the question: How can artificial superselectivity be accomplished in synthetic cell membrane mimics? Not only is this important to expand the understanding of biological systems, but also to develop synthetic protocells with life-like function. I will introduce our concept for superselectivity in synthetic cell membranes which requires the integration of (i) specificity, (ii) multivalency (to enhance binding but retain reversibility), (iii) 2D dimensional organization of receptors and (iv) concepts of cooperativity in binding. To tackle this my team has designed and synthesized new families of amphiphiles —comb-polymers and Janus dendrimers— that self-assemble into cell-mimetic vesicles. Although, these molecules do not exist in nature, the vesicles formed closely mimic the thickness, flexibility, and lateral 2D organization of cell membranes. These properties are precisely encoded in the chemical structure, architecture and topology of the macromolecular building blocks of the membrane. As an example, I will show our recent work where we discovered that the reactivity of sugar receptors towards lectins is enhanced by the 2D organization of sugars into nanoarrays (clustering) and raft-mimics (cooperativity) on the periphery of protocells.[1] Furthermore, this talk will show how to introduce life-like functions such as endocytosis of living bacteria without active cell machinery.[2]

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Aligns with meeting schedule

ON THE AMYLOID WORLD HYPOTHESIS

Saroj K. Rout, **Radoslaw Bomba, Michael P. Friedmann, Witold Kwiatkowski, Jason Greenwald & Roland Riek**

Laboratory of Physical Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich

How can simple molecules become organized into complex systems capable of supporting life? To address this question we have turned to small peptides that are capable of aggregating into beta-structured amyloids. We hypothesize that amyloids could have helped bridge the complexity gap that lies between small <200 Da prebiotic molecules and ordered macroscopic structures of the kind that can support catalytic and self-replicative functions. The projects described in this poster have revealed numerous activities and characteristics of amyloids, ranging from their feasibility as prebiotic entities and their effect on the chiral amplification of polymerizing amino acids to their ability to catalyze reactions and template their own replication. The cooperative interactions between amyloids and other (pre)biological molecules such as vesicle-forming fatty acids have also been investigated, providing insights into the formation of early membranes. Work by others on the cooperative assembly of amyloid and nucleic acid suggest that amyloids are capable of acting as a template for other polymers, suggesting a possible early connection between the peptide and RNA pre-biotic worlds. Amyloids, with their uniquely repetitive and templating structure, exceptional stability, chiro-selectivity, catalytic ability could have played important roles in the dynamic processes on the prebiotic earth that led to the increased complexity, organization and compartmentalization of key molecules and, eventually life.

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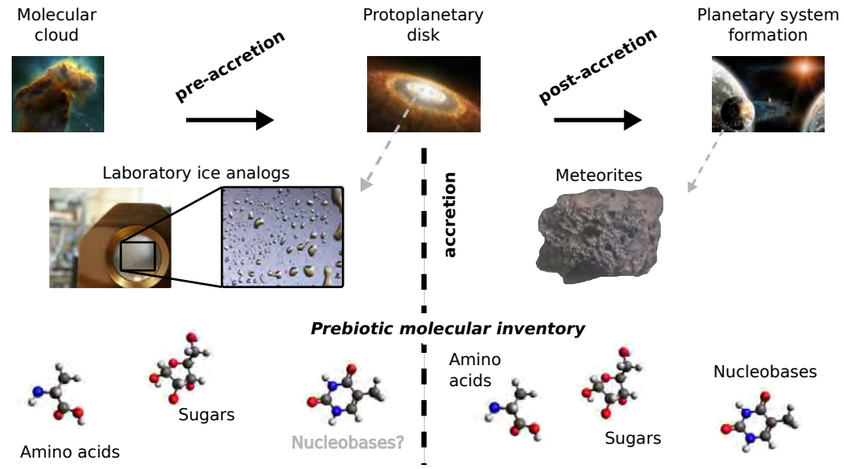

THE CHALLENGING DETECTION OF NUCLEOBASES FROM PREACCRETIONAL ASTROPHYSICAL ICE ANALOGS

Alexander Ruf[1], **Justin Lange[2], Balkis Eddhif[2], Claude Geffroy[2], Louis Le Sergeant d'Hendecourt[1], Pauline Poinot[2], and Grégoire Danger[1]**

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Amino acids, sugars, and nucleobases are considered as the so-called molecular bricks of life, the major subunits of proteins and genetic materials[1]. All three chemical families have been previously detected in meteorites[2]. In dense molecular cloud ice analogs, the formation of a large set of amino acids and sugars (+derivatives) has been observed[3,4]. In this contribution, we demonstrate that similar ices (H_2O:$^{13}CH_3OH$:NH_3 ices, 2:1:1) can also lead to the formation of nucleobases[5]. Using combined UPLC-Orbitrap mass spectrometric and UPLC-SRM-triple quadrupole mass spectrometric analyses, we have unambiguously detected cytosine in these primitive, realistic astrophysical ice analogs. Additionally, a huge variety of nucleobase isomers was observed. These results indicate that all central subunits of biochemical materials may have already been present at early stages of chemical evolution of the protosolar nebula, before accretion toward planetesimals. Consequently, the formation of amino acids, sugars, and nucleobases does not necessarily require secondary alteration processes inside meteoritic parent bodies. They might have been supplied from dense molecular cloud ices toward post-accretional objects, such as nonaqueously modified comets, and subsequently delivered onto the early Earth's surface, potentially triggering the emergence of prebiotic chemistry leading to the first living systems.

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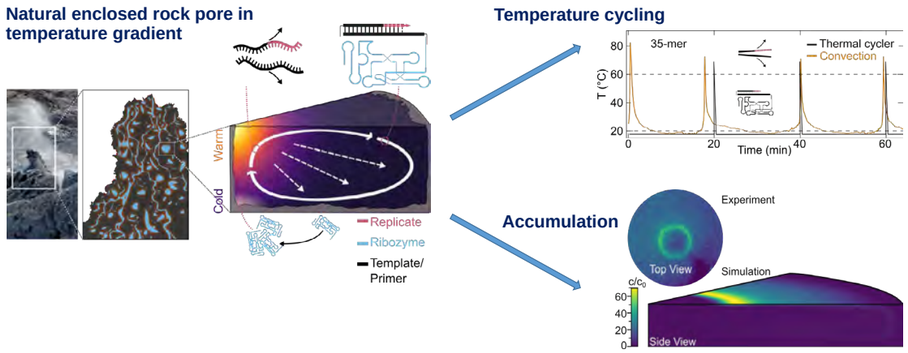

A THERMAL HABITAT THAT TRIGGERS THE RETENTION AND RNA-CATALYZED REPLICATION OF RNA

Annalena Salditt[1], **David P. Horning[2], Lorenz M. R. Keil[1], Christof B. Mast[1], Gerald F. Joyce[2] & Dieter Braun[1]**
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Early replication in the RNA world is assumed to be an RNA-catalyzed process. In vitro evolution provided ever better RNA-based polymerases, but the required strand separation as well as the emergence of these complex ~200-base catalytic sequences are unsolved questions for the Origin of Life.

Here, we present a microfluidic reaction compartment with a pointed heat source, that both protected and drove laminar thermal convection in aqueous solution and allowed the autonomous, exponential RNA amplification by the RNA strand separation. The reaction proceeded despite the instability of RNA at elevated temperatures under the required salt conditions and offered replication kinetics comparable to explicit thermal cycling.

Accumulation experiments with fluorescently labeled nucleic acids revealed a ring like accumulation pattern for the long functional RNA-polymerase as well as its DNA complement, whereas similar experiments for dsDNA of similar length showed the expected central accumulation. Imaging the reaction mixture at higher resolution revealed the formation of micrometer sized conglomerates that depended on presence of PEG, introduced as crowding agent in the buffer. By including a diffusiophoretic term, the experimental accumulation behavior could be matched by simultaneously simulating the accumulation of the conglomerates and PEG with a commercial finite element simulation code.

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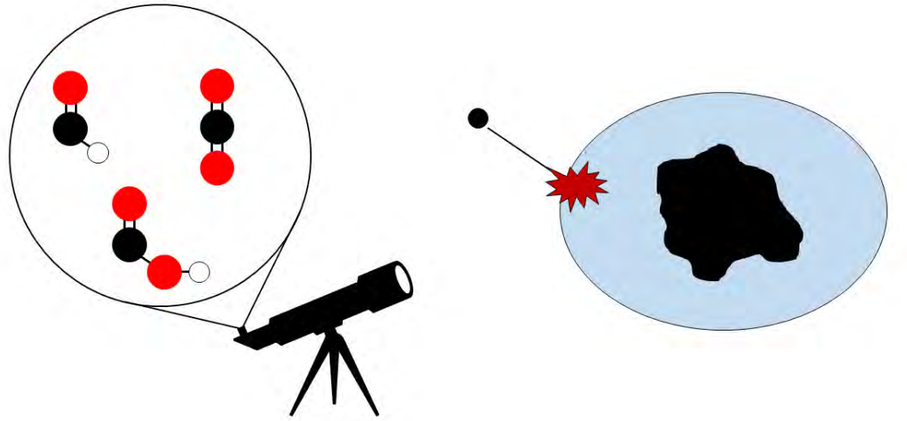

THE ORIGIN OF INTERSTELLAR CO_2

Fabian Schmidt, **Jan Hendrik Bredehöft**
Universität Bremen, Institut für Angewandte und Physikalische Chemie

Carbon monoxide (CO) and carbon dioxide (CO_2) are some of the most abundant molecules in the icy mantles around interstellar dust grains[1]. Unlike many other abundant molecules, CO_2 cannot be formed by gas phase reactions, as the newly formed bond immediately dissociates without a third body to remove excess energy[2]. While it is commonly accepted, that CO_2 forms from energetic processing of CO and water (H_2O) in the ice phase, the exact mechanism of the reaction is less well known. One major point of contention is the role of the intermediate hydrocarboxyl radical ($HOCO^{\bullet}$) whose presence in the reaction mixture has been clearly shown by infrared spectroscopy[3]. Theoretical models predict, however, that $HOCO^{\bullet}$ should not be able to form CO_2 by dissociation of its O-H bond[4], for energetic reasons.

It is known, that energetic processing of a H_2O:CO mixture does not only produce CO_2, but also formic acid, formaldehyde and methanol[3].

In the present poster, we present results of a further experimental investigation, looking at the H_2O:CO system under energetic processing with low-energy electrons (2-20 eV)[5]. By looking at the dependence of product yield on electron energy, it is possible to unravel what kind of primary electron-molecule interaction starts a reaction sequence and which products are formed from specific intermediates. We observe that $HOCO^{\bullet}$ is indeed an important intermediate, just not on the reaction path to CO_2, but as a precursor to formic acid. CO_2, on the other hand is formed by dissociation of H_2O into neutral O atoms and H_2.

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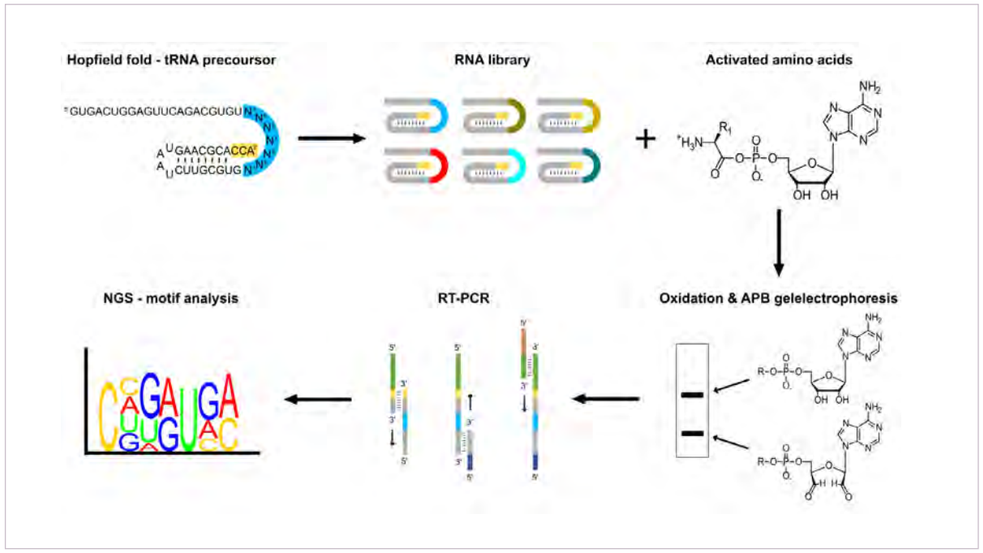

RNA LIBRARY SCREENING FOR SELF-AMINOACYLATING TRNA PRECURSORS

Christian Schmitt, **Andres Jäschke1**
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In every modern organism, protein biosynthesis follows the same principle: codons, which consist of three bases of genetic information encode one specific amino acid. This genetic code is basically identical throughout all kingdoms of life. Transfer RNAs (tRNAs) carry complementary anticodons which facilitate the translation of these codons into chains of amino acids i.e. proteins. But proteins are also needed to load the tRNAs with their corresponding amino acid. This resembles a chicken or egg problem for the beginning of life and even though this problem is well known to the scientific community, there is little experimental data available. This project specifically addresses the 'testable Hypothesis' formulated by J. J. Hopfield in 1978[1]. His postulated Hopfield folds resemble tRNA precursors in which the anticodon can directly interact with the amino acid attachment site. Unlike modern tRNAs should these precursors be able to bind specific amino acids on their own depending on the sequence of their anticodon. In this project, the hypothesis will be tested through kinetic sequencing of RNA libraries. The libraries consist of Hopfield folds with randomized anticodons and will be mixed with activated amino acids. Upon oxidation with periodate, APB gel electrophoresis, reverse transcription and reduced cycle PCR, DNA libraries are being created which are sequenced by next generation sequencing techniques. The sequencing data may show reproducible enrichments of certain sequences depending on which amino acid was used. This will not only show if such a precursor was practically possible but also how the genetic code itself was initially defined.

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CATALYTIC PEPTIDES - POTENTIAL PRECURSORS OF ENZYMES?

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[2] Eindhoven University of Technology, Institute for Complex Molecular Systems, Het Kranenveld, 5600 MB Eindhoven , The Netherlands.

Nature uses enzymes to catalyze reactions essential for life. The complexity of enzymes is thereby crucial for their reactivity, stereo- and chemoselectivity. In recent years numerous small peptidic catalysts were developed that have high levels of reactivity and stereoselectivity.[1] These peptides are smaller and less complex than enzymes but show features reminiscent of enzymes. Moreover, peptides and enzymes are buildup of the same building blocks: amino acids. This provokes the question of a potential role of catalytic peptides in the evolution of enzymes. Based on a combinatorial library screening with more than 3000 peptides, our group developed tripeptidic catalysts of the H-Pro-Pro-Xaa type (Xaa: any amine). These peptides are highly reactive and stereoselective catalysts for aldol and conjugate addition reactions in organic solvents and water.[2] Underlying reaction mechanisms as well as conformational features of the peptides are well understood.[3] Hence, H-Pro-Pro-Xaa type catalysts are ideal model systems to explore a potential role of catalytic peptides in the evolution of life. Here, we address two related questions: 1) There is a general notion that the bigger and more complex peptidic catalysts are, the more enzyme-like and better they should become. But is this really true?[4] 2) A prerequisite for a potential role of peptides in the evolution of enzymes is high chemoselectivity. Yet, are peptidic catalysts robust enough to perform reactions in complex multi-component environments?[5]

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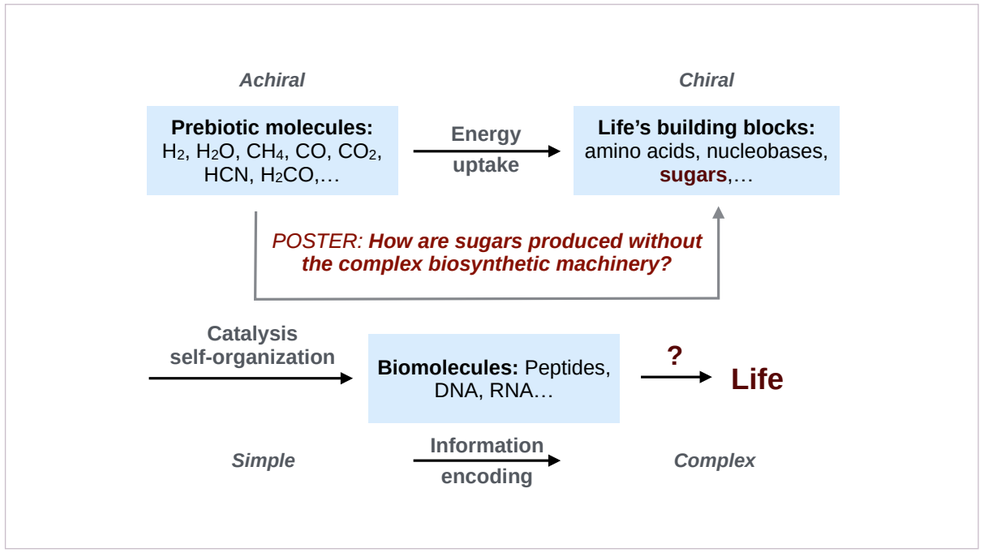

CARBOHYDRATE FORMATION IN THE ABSENCE OF BIOSYNTHESIS

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Although the simplest sugar, glycolaldehyde ($HOCH_2CHO$), has been generated in the lab from its constituents[1] and is suggested to occur in the formose[2] (Butlerow[3]) reaction, the mechanism for the dimerization of two H2CO molecules to glycolaldehyde and on to higher sugars is a riddle to date; the finding of "glycolaldehyde autocatalysis" does not explain the fundamental chemistry, requires the presence of liquid water, a strong base, high reactant concentrations, and ambient temperatures – all conditions unlikely to be present on early Earth or in extraterrestrial environments.[4] We focus on non-aqueous reactions, ideally starting directly from the photoreaction of CO and H_2 to give hydroxymethylene (HCOH)[5]: Under appropriate conditions H_2CO and HCOH react to glycolaldehyde and glyceraldehyde.[6] Similarly, we demonstrate that glycolaldehyde and H_2CO form a new 1,3-dioxolane that may well be the photostable storage form of these two key molecules.[7] Finally, with "time-compression experiments" we demonstrate the formation of glyoxylic acid from the HCO and HOCO radicals under conditions mimicking those of interstellar water ices doped with CO.[8]

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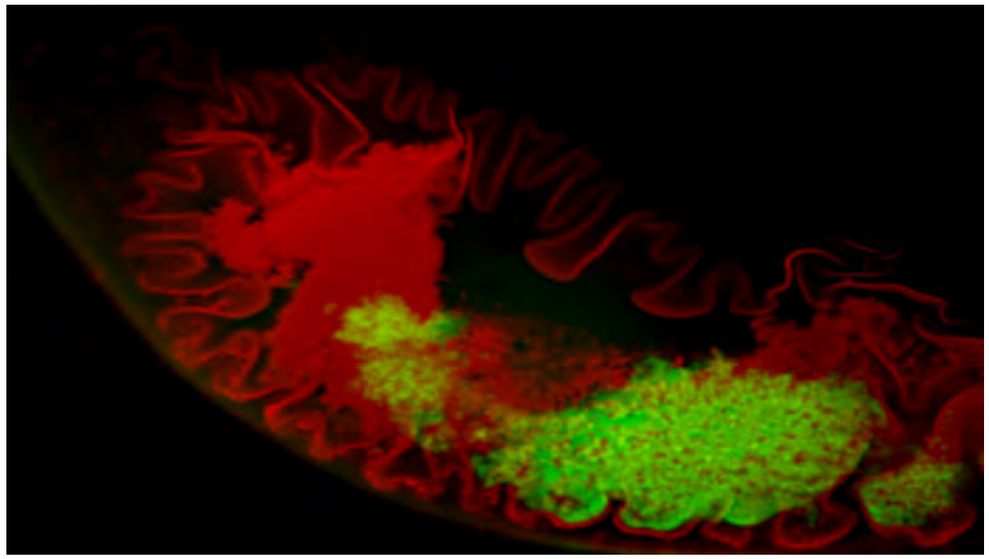

THERMAL GRADIENT DRIVEN FORMATION OF HOMOCHIRAL DOMAINS IN HYDROGELS STARTING FROM RACEMIC POLYNUCLEOTIDE MIXTURES

Philipp Schwintek, **M. Heinlein, C. Mast and Dieter Braun**
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The origin of homochirality of DNA still remains an unresolved puzzle for the origin of life research[1]. In previous work, the formation of DNA-hydrogels inside porous rock of hydrothermal vents has proven to be sequence specific[2]. This work investigates the selectivity of such hydrogels towards DNA-backbone enantiomers, forming homochiral domains starting from racemic solutions. Mimicking boundary conditions similar to hydrothermal pores as well as using real time fluorescent microscopy enables us to monitor the accumulation of DNA molecules in situ.
By screening parameters such as salt concentrations, temperatures, DNA-sequences and pore-geometries, we investigate the phase-separation into hydrogels as a darwinistic selection pressure that could have led towards homochirality of biopolymers.

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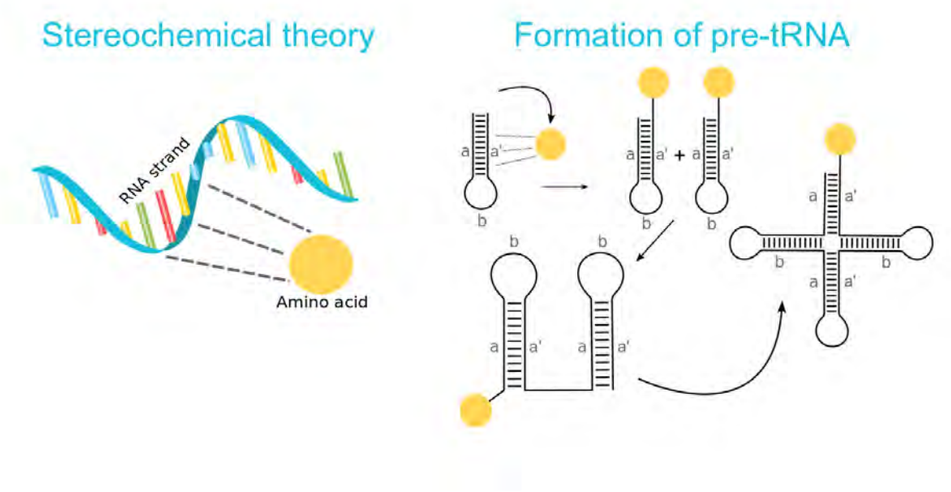

UNDERSTANDING THE GENETIC CODE FROM AFFINITIES OF AMINOACYL ADENYLATES TO PRE-TRANSFER RNA MOTIFS

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The patterns present in the genetic code and its wide conservation across species suggest that it was not a random accident. According to the stereochemical theory, assignments between codons and amino acids originated from intrinsic interactions between RNA and amino acids or small peptides. RNA/Amino acid complexes could have played a role in translation from the beginning, or could have initially acted as cofactors for ribozymes or as nucleic acid stabilizers.
In 1978, J.J Hopfield proposed a potential primordial secondary structure for the tRNA in which the anticodon loop is placed in direct vicinity of the CCA end, which is a strong argument in favor of the stereochemical theory. As a starting point for the experimental validation of this theory, we are testing double stranded RNA complexes, based on the pre-tRNA structure proposed by Hopfield, and measuring their binding affinities to AMP and activated amino acid analogs.
The binding affinity constants of the designed constructs to AMP are on the milimolar range. The next step consists of measuring the binding affinities of the corresponding activated amino acid analogs. We are interested in finding specific binding of the amino acid moieties to the constructs 'anticodon' overhang, which would reflect on a stronger binding. This could shed a light on the origin of the present day correspondence between codons and amino acids.

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SUGARS PROGRAM THE HIERARCHICAL SELF-ASSEMBLY IN ONION GLYCODENDRIMERS

D. Söder[1], **N. Yu. Kostina[1], T. Haraszti[1], K. Rahimi[1], Q. Xiao[2,3], M. L. Klein[3], V. Percec[2], C. Rodriguez-Emmenegger[1]**
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[2] Roy & Diana Vagelos Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, United States
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Natural cell membranes contain nano- and micro-organized domains formed by non-random association of lipids. Located at the cellular interface these functional domains contain glycoproteins and glycolipids that control functions such as communication, division, cargo trafficking, and signal transduction. The sugar moieties provide the structural basis for affinity in protein recognition and the formation of molecular patterns on the surface. But can these patterns be controlled by the sugar type? And how do these nanoarrays affect the binding of lectins, the cell-binding proteins? In this poster I tackle these questions with the help of Janus glycodendrimers (JGDs). Recently, we reported the self-assembly of JGDs into cell membrane-mimics in water, named glycodendrimersomes (GDSs).[1] The resulting uni- and multilamellar vesicles closely resemble the thickness, flexibility and lateral 2D organization of natural cell membranes.[2] These properties stem from the chemical structure, architecture, and topology of the dendrimer. For this study, the JGDs are decorated with the monosaccharide mannose (Man). Man is highly biologically relevant. We demonstrated an increase in the biological activity of sugars when they formed nanoarrays. We discovered that the co-assembly of judiciously selected Janus dendrimers (JDs) with JGDs led to multiscale membrane architectures. AFM allowed observing how dendrimers segregated in micrometer-size raft-like domains with the Man moieties nano-assembled in lamellar or hexagonal patterns. These periodic arrays of Man resulted in a new ligand with enhanced reactivity to Concanavalin A as determined by surface plasmon resonance. Thus, these experiments provide a powerful example in which structure determines function, in particular how different supramolecular assemblies encode biological recognition.

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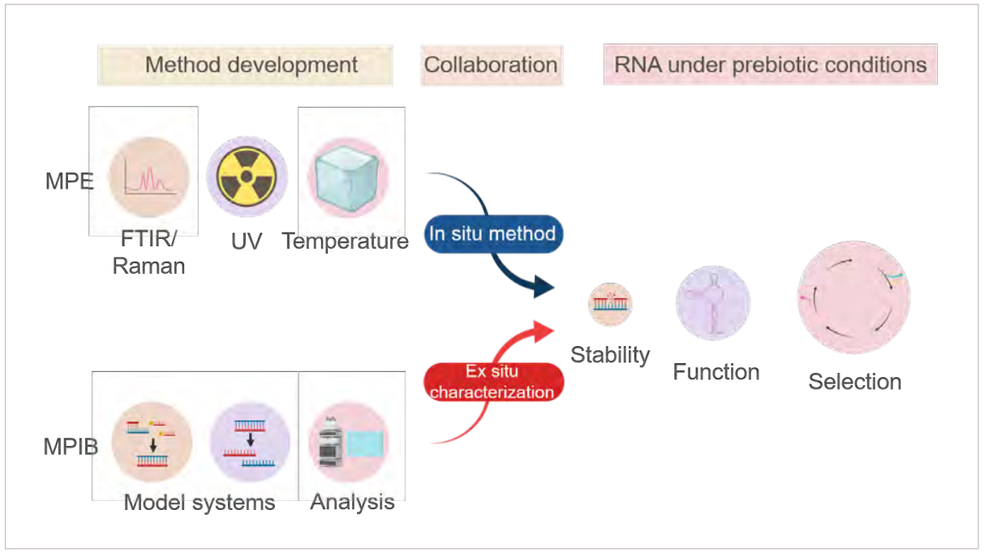

PROBING RNA STABILITY, FORMATION, & CATALYSIS IN SIMULATED PREBIOTIC ENVIRONMENTS ON THE EARLY EARTH AND IN SPACE

Emilie Y. Song[1], **Max Winkler[2], Paola Caselli[2], Hannes Mutschler[1]**
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Can life based on nucleic acids survive and evolve in extreme, precellular conditions provided by early Earth or even space? Given the lack of spatiotemporal data of abiogenesis, a wide range of conditions provide possible prebiotic environments including hydrothermal vents[1], impact craters[2], ice[3], and warm ponds[4]. We aim to reduce the number of these possible environments by systematically narrowing down the range of physicochemical parameters that allow the sustained emergence and/or existence of biopolymers. Specifically, we focus on ribonucleic acid (RNA) polymers and building blocks, which are thought to be central key players in early chemical and Darwinian evolution[5]. We employ a powerful reaction setup capable of simulating relevant prebiotic environmental conditions such as the young Sun UV spectrum. Using this setup, we characterize RNA survival, synthesis, and catalysis under realistic conditions using methods such as Raman spectroscopy, HPLC, electrophoresis, and deep sequencing to explore to what extent RNA molecules are capable of survival, adaptation and evolution in extreme environments.

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Aligns with meeting schedule

PREBIOTIC SYNTHESIS IN VOLCANIC DISCHARGES: AN EXPERIMENTAL APPROACH

Christina Springsklee[1], **Thomas Steiner[2], Thomas Geisberger[2], Bettina Scheu[1], Claudia Huber[2], Wolfgang Eisenreich[2], Corrado Cimarelli[1], and Donald Bruce Dingwell[1]**

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The formation of primitive organic molecules is a key question in the enigmatic debate on the emergence of life on Early Earth. Several iconic experiments already explored potential processes which lead to the formation of organic molecules. One of these experiments are the discharge experiments performed by Miller and Urey, which corroborates the conclusion that amino acids can be produced by lightning under reducing atmospheric conditions[1].

This project aims to combine prebiotic discharge experiments with a geological relevant setting for Early Earth: active volcanism. For this purpose, a shock tube apparatus was developed to perform discharge experiments in varying atmospheres. The discharges are generated by the eruption of the volcanic ash itself by triboelectrification and fracto-emission, a process which is frequently observed in nature and described as volcanic lightning. In the experiment the total magnitude of electric discharge can be adjusted by changing the amount of mass of ash, the proportion of fines and eruptive conditions[2]. The development of the new experimental setup allows to probe the ejected sample, the gas atmosphere, present before and after the experiment, as well as to quantify the magnitude of total discharge generated during the experiment. Special focus is given to the role of ash, offering variable porosity, high surface area and significant surface reactivity. This project aims to determine and quantify the impact of volcanic ash on its environmental setting as a catalyst and a container in the creation and accumulation of first organic molecules.

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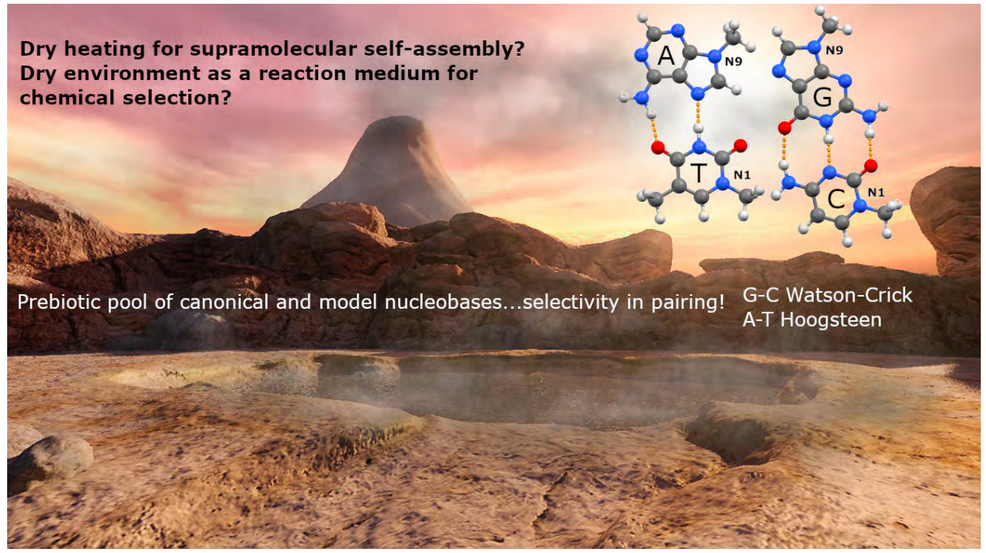

THE SOLID-STATE AS A REACTION MEDIUM FOR PREBIOTIC CHEMICAL SELECTION: DRY HEATING ENABLES SELECTIVE PAIRING OF MODEL NUCLEOBASES

Tomislav Stolar[1], **Martin Etter[2], Krunoslav Užarević[1], Ivan Halasz[1], Ernest Meštrović[3]**

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From the perspective of prebiotic DNA assembly, it seems unlikely that the specific pairs of nucleobases would have been coupled into DNA if they were unwilling to selectively and specifically self-assemble beforehand[1]. Base pairing of canonical nucleobases, or their simple derivatives, is known to be notoriously difficult to achieve in aqueous media, due to solvation issues and competition for hydrogen bonding[2]. Here, we show that pairing of methylated guanine and methylated cytosine is readily achievable by dry heating of their solid mixtures[3]. In the G-C cocrystal, molecules self-assemble in the Watson-Crick hydrogen-bonded motif. Furthermore, selectivity in the solid-state self-assembly is DNA-specific. Dry heating of a four-component mixture of methylated adenine, guanine, cytosine, and thymine provided only A-T and G-C pairing. Equivalent experiments with canonical nucleobases failed to yield pairing, and there seems to be a strong influence of the methyl group at the glycosidic nitrogen atom. The findings of this study suggest that chemical processes occurring in the solid-state could have had an important role in the prebiotic chemistry context. For our future endeavors, we will include a larger pool of proto-nucleobases[4,5].

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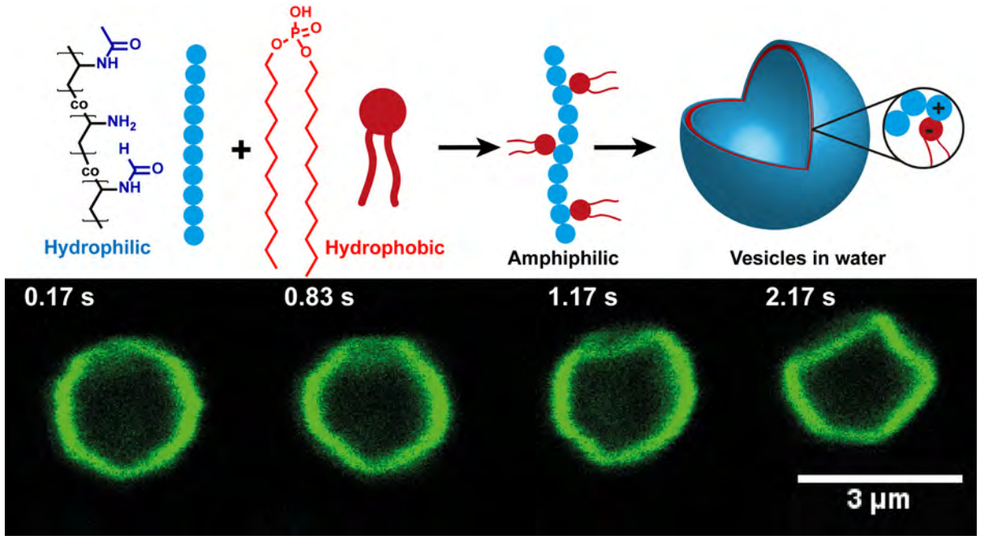

SUPER-FLEXIBLE BIOMIMETIC VESICLES

Jan Tenbusch, **Pilar Bologna, Nina Kostina, Mehrnoush Rahimzadeh, Khosrow Rahimi, Cesar Rodriguez-Emmenegger**
DWI – Leibniz Institute for interactive Materials e.V. Aachen

Compartmentalization is essential to life. As protocellular research – and the study of abiogenesis – was driven forward in the last couple decades, researchers had to tackle different obstacles. Stability and longevity in cell membrane models are achieved by either utilizing cholesterol in high molar ratios when working with liposomes, or polymersomes assembled from block copolymers. Both approaches present their own disadvantages such as a low 2D mobility and storage problems for the former and no biomimetic thickness as well as a low flexibility and 2D mobility for the latter. In this poster we will present a new class of amphiphiles that are able to self-assemble into super-flexible biomimetic vesicles. We designed and synthesized non-covalently linked amphiphilic comb-shaped oligomers which amalgamate the stability of polymersomes with the biomimetic properties of liposomes while increasing the flexibility many times over. A flexible intrinsic hydrophilic oligomer backbone is utilized to which alkyl chains are attached by ionic interactions. The length of the alkyl chains is selected to represent the biomimetic thickness of the natural cell membrane (5±1 nm). We control the degree of flexibility by encoding the grafting density of the alkyl chains along the hydrophilic backbone. These molecules create new possibilities for applications where high dynamics of the membrane are necessary.

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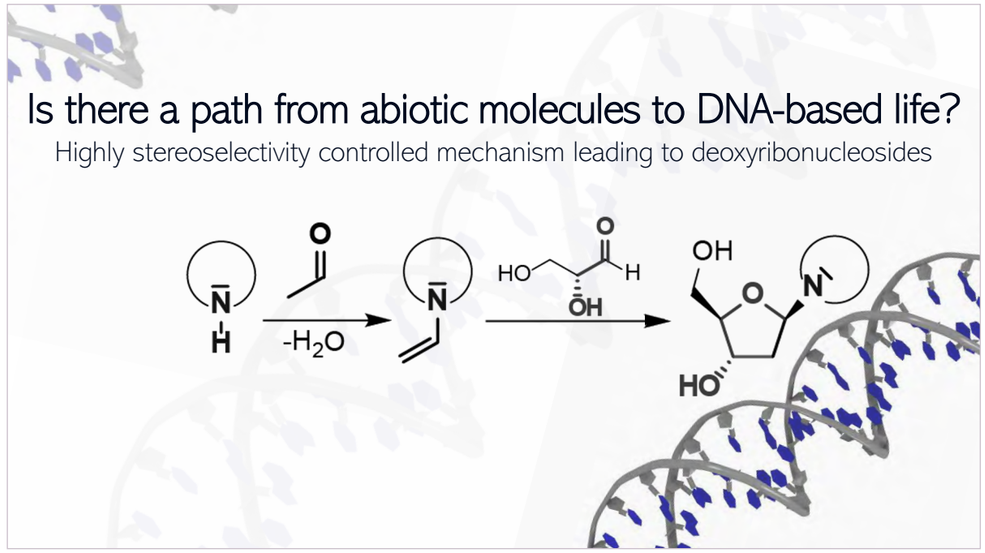

PREBIOTIC PATHWAY TO DNA NUCLEOSIDES

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So far it is assumed that RNA played a key role in the origin of life. However, the transition from ribonucleotides to deoxyribonucleotides remains unknown.[1] Therefore, the question remains: Is there a path from abiotic molecules to DNA-based life?
We are exploring the formation of deoxyribonucleosides under relevant prebiotic conditions in water in high regio- and stereoselectivity from adenine, guanine, cytosine, and thymine. By condensation of the canonical bases with acetaldehyde and sugar-forming precursors we found a continuous path to deoxyribonucleotides, starting from prebiotically available molecules.[2,3] The experimental studies are complimented with computational simulations to elucidate aspects which are experimentally inaccessible.

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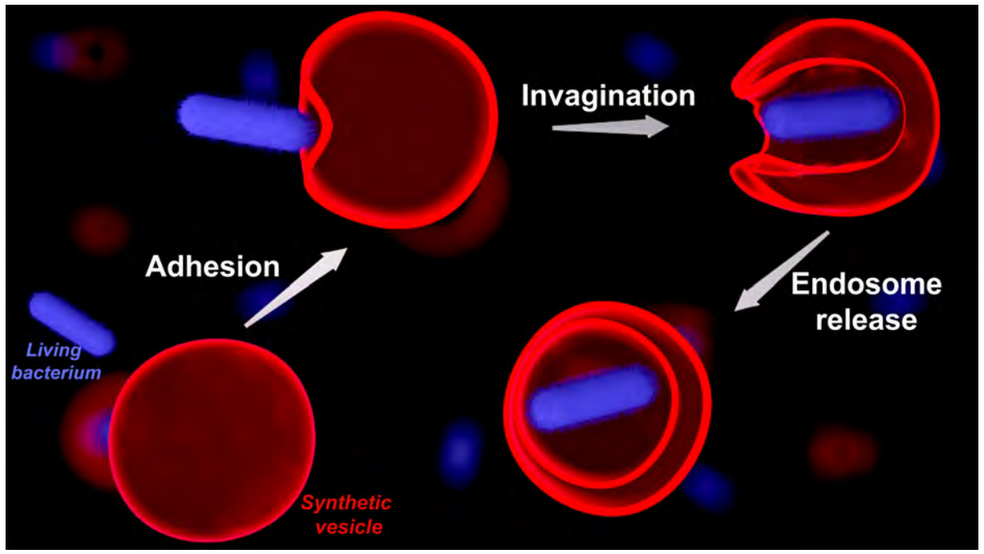

BUILDING MEMBRANE MACHINES TO ENDOCYTIZE LIVING BACTERIA: THE BATTLE BETWEEN ADHESION AND FLEXIBILITY

Mariia Vorobii, **Nina Kostina, Jan Tenbusch, Tamas Haraszti, Mehrnoush Rahimzadeh, Dominik Söder, Virgil Percec, Cesar Rodriguez-Emmenegger**
DWI – Leibniz Institute for Interactive Materials e.V., RWTH Aachen UniversityDepartment of Physics, LMU Munich

There is much interest in developing vesicular microcompartments from natural and synthetic amphiphiles, enabling programmable interactions with living matter. Of particular interest is the development of vesicles capable of endocytosis of living bacteria. Despite the complexity of this process, theoretical studies predict that the endocytosis of prolate micro-objects is possible without the need of active cell machinery if the energy released upon bacterial adhesion to the membrane surpasses the energy required to bend the membrane. Nonetheless, natural liposomes and synthetic polymersomes fail to sufficiently recapitulate membrane properties to perform this advanced function. Here we report the engulfment of living bacteria into endosomes by cell-like dendrimersomes assembled from Janus dendrimers.[1] Full engulfment occurred in less than a minute after contact. The process is driven by the adhesion of the bacterium to the dendrimersome's membrane by ultraweak interactions, comparable to those utilized by nature. The key to success relies on the combination of high flexibility and stability of the dendrimersomes. The key properties of the dendrimersomes are programmed into the molecular structures of their building blocks. The ability to support endocytosis highlights opportunities for the design and programming of dendrimersomes in biomedical research.

1 Kostina, N. Y.; Rahimi, K.; Xiao, Q.; Haraszti, T.; Dedisch, S.; Spatz, J. P.; Schwaneberg, U.; Klein, M. L.; Percec, V.; Moller, M.; Rodriguez-Emmenegger, C., Membrane-Mimetic Dendrimersomes Engulf Living Bacteria via Endocytosis. Nano Lett 2019, 19 (8), 5732-5738.

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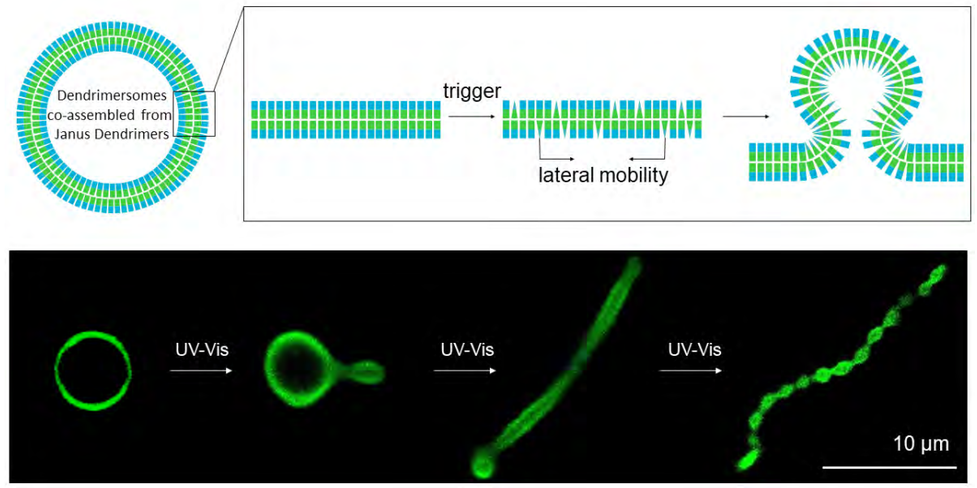

HOW DOES SPONTANEOUS CURVATURE INDUCE THE MORPHOGENESIS OF DENDRIMERSOME VESICLES?

A. M. Wagner, **N. Y. Kostina, T. Haraszti, K. Rahimi and C. Rodriguez-Emmenegger**
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The vital functions of cell membranes require their ability to quickly change shape to perform complex tasks such as motion, division, endocytosis, and apoptosis. Membrane curvature in cells is modulated by very complex processes such as changes in lipid composition, the oligomerization of curvature-scaffolding proteins and the reversible insertion of protein regions that act like wedges in the membrane. But, could a much simpler mechanism support membrane shape transformation? In this poster, I will show how the change of the amphiphile topology (shape) in the bilayer can drive the morphogenesis of cell membrane models. To tackle this, we have designed and synthesized a new type of amphiphiles —Janus dendrimers— that self-assemble into uni- or multilamellar vesicles.[1] Although these molecules do not exist in nature, the vesicles formed closely mimic the thickness, flexibility and the lateral 2D organization of cell membranes. These properties are precisely encoded in the chemical structure, architecture, and topology of the macromolecular building blocks of the membrane.[2] For these studies, we synthesized Janus dendrimers containing a photo-labile bond that upon UV-irradiation cleave losing a part of the hydrophilic dendron. This leads to a change from a cylindrical to a wedge-shaped amphiphile. The high mobility of these dendrimers allows for the concentration of the wedge-shaped amphiphiles and the generation of local spontaneous curvature. The concentration of the wedges and their rate of segregation allowed controlling the budding and generation of structures such as tubules, starfish, and high genus vesicles.

1 C. Rodriguez-Emmenegger, et al, Proc Natl Acad Sci U S A 2019, 116, 5376-5382.
2 N. Kostina, K. Rahimi, Q. Xiao, T. Haraszti, S. Dedisch, J. P. Spatz, U. Schwaneberg, M. L. Klein, V. Percec, M. Moeller, C. Rodriguez-Emmenegger, Nano Lett 2019, 10.1021/acs.nanolett.9b02349.

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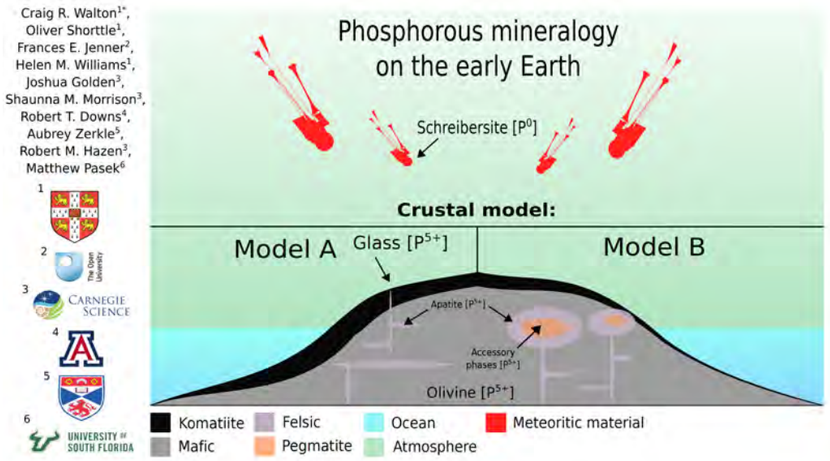

PHOSPHOROUS MINERALOGY ON THE EARLY EARTH

Craig R. Walton[1], **Oliver Shorttle[1,2], Frances E. Jenner[3], Helen M. Williams[1], Joshua Golden[4], Shaunna M. Morrison[5], Robert T. Downs[4], Aubrey Zerkle[6], Robert M. Hazen[4], Matthew Pasek[7]**

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It has long been held that the early crustal phosphorous (P) reservoir was dominated overwhelmingly by apatite ($Ca(PO_4)_3OH,Cl,F$). The relative insolubility of apatite under ambient surface conditions today presents a challenge to the early availability of phosphate with which to drive prebiotic chemistry and sustain early life. However, stark differences in P mineralogy are found between mafic and felsic rocks. Given that global crustal compositions have evolved towards more felsic compositions over time, we might expect a contemporaneous evolution in crustal P mineralogy. We critically examine the evidence for a such a shift, beginning with a review of the processes that lead to the formation of the Earth, moving through the delivery of exogeneous P to the Earth's surface, and exploring the possible makeup of P mineral reservoirs in the early emergent crust. We conclude that exogeneous schreibersite, along with crustal silicate-hosted P (olivine, pyroxene, and glass), and terrestrial apatite were dominant on the early Earth. However, apatite was likely a much more minor phase in the early crust, in particular during the Prebiotic Era, than has been previously assumed (< 50 %, potentially as low as < 1 %). Silicate weathering may have played a vital role in supplying prebiotic chemistry and early life with available phosphate.

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PUBLIC OUTREACH ON EMERGENCE OF LIFE

Karl Wienand, **Wolfgang M. Heckl1, CRC 235 Collaboration**
Deutsches Museum, Museumsinsel 1, 80538 Munich, Germany

Research on the emergence of life has the potential to captivate a large public, but is often little known. Involving scientists, especially junior scientists, could improve the communication and the public understanding of this important field of research[1].
The Collaborative Research Center 235 Emergence of Life[2] puts a strong emphasis on outreach. Its planned effort includes a number of initiatives—from public talks to events in schools. It will culminate in the realization of a museum exhibition about the science and research on emergence of life. Participating researchers (especially PhD students) actively participate in ideating, designing, and realizing the exhibition and all other outreach activities.
In this poster, I will present some contents currently in the works, both for the exhibition and for more general outreach.

1 D. Battachary. Survey of Factors Affecting Science Communication: Conclusions, Recommendations and Actions. Royal Society, 2006.
2 https://www.emergence-of-life.de

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UV RESISTANCE OF NUCLEOSIDES - AN EXPERIMENTAL APPROACH

Max Winkler, **Barbara Michela Giuliano, Paola Caselli**
Max Plank Institute for Extraterrestrial Physics

The emergence of life on Earth is a highly discussed, but still unsolved question. Different hypotheses have been proposed. Current research underlines the importance of environments within close proximity to the Earth's surface as they can solve long standing problems like polymerisation of nucleotides[1] and phosphorylation of nucleosides[2]. However, surface-near settings, e.g. ponds or ice shields, are prone to UV irradiation. We investigated the photosensitivity of uracil, uridine, adenosine, cytidine and guanosine by using Raman microscopy. DMSO was used as a solvent to improve the signal to noise ratio. The samples were irradiated by a UV source with 150 mW/cm² for 10 minutes. Uracil and uridine showed the highest photosensitivity, while adenosine, cytidine and guanosine remained stable. This stands in contradiction with previews works using ab initio quantum calculations[3]. These studies concluded that uracil is more photostable than the other canonical nucleobases. However, theoretical investigations suffer from limitations and simplifications, e.g. intermolecular interaction or their photo cross sections, due to high computational costs. This could explain the observed lower UV resistance of uracil and uridine. Understanding the survivability of these important biomolecules is important to understand the prebiotic chemistry of the early Earth. Environmental stresses could have served as drivers towards a rise in chemical complexity.

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FLOOR 10

ACID-CATALYZED POLYMERIZATION OF CYCLIC GMP

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[2] Institute of Biophysics, Academy of Sciences of the Czech Republic, Královopolská 135, Brno 61265, Czech Republic

Different prebiotic pathways have been explored for the synthesis of nucleosides and nucleotides, yet our current understanding lacks in deciphering a prebiotically plausible route for their polymerization to form long linear oligonucleotides. Methods involving activation chemistry of nucleotides in aqueous solutions are not only challenging due to different side reactions, but gives rise to the question whether such activating agents existed on prebiotic Earth. Cyclic nucleotides have been shown to be a viable precursor in prebiotic polymerization[1]. It has been demonstrated previously that 3'-5' cGMP, in its free acid form, can spontaneously polymerize under hot and dry conditions by transphosphorylation of the phospohodiester bond[2]. We demonstrate that the Na-salt of cGMP, which does not polymerize upon drying in alkaline conditions, can be polymerized under acidic conditions. Therefore, in addition to previously described base-catalyzed reaction mechanism[3,4], we propose and motivate an alternative acid-catalyzed mechanism for the ring opening polymerization of cGMP.

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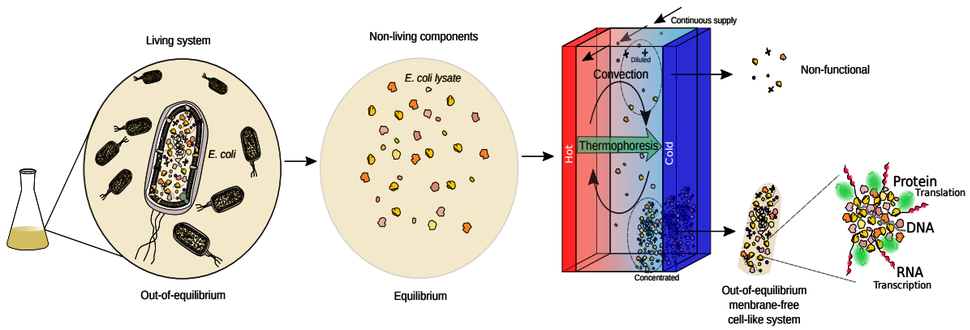

OUT-OF-EQUILIBRIUM CELLULAR MIMICS DRIVEN BY THERMAL GRADIENTS

Noël Yeh Martín[1], Laura Weise[2], Hannes Mutschler[2], Sheref Mansy[3,4], Christof Mast[1] & Dieter Braun[1].

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Thermal gradients applied at the microscale have been shown to accumulate diluted simple mixtures of molecules to high local concentrations[1-3]. It is unclear, however, whether thermal gradients could also drive complex biochemical reactions. In other words, it is yet to be assessed whether vastly different biomolecules in complex mixtures can be accumulated together into a cooperative and functioning system that could display the properties of a living cell. Therefore, we are currently exploring the feasibility of exploiting thermal gradients to generate a disequilibrium system reminiscent of natural living cells by accumulating the hundreds of components of an E. coli cell lysate[4] and the purified components of PURE system[5] needed to reconstitute RNA and protein synthesis in the absence of a membrane comparment. Furthermore, we are aiming at sustaining the activity of our system over long periods of time by a continuous supply of feedstock molecules and removal of waste toxic products that would lead to a long lasting cell like system operating under disequilibrium. Ultimately, we hope that our approach will help us gain insight of the fundamental processes and the set of conditions needed to sustain cellular life.

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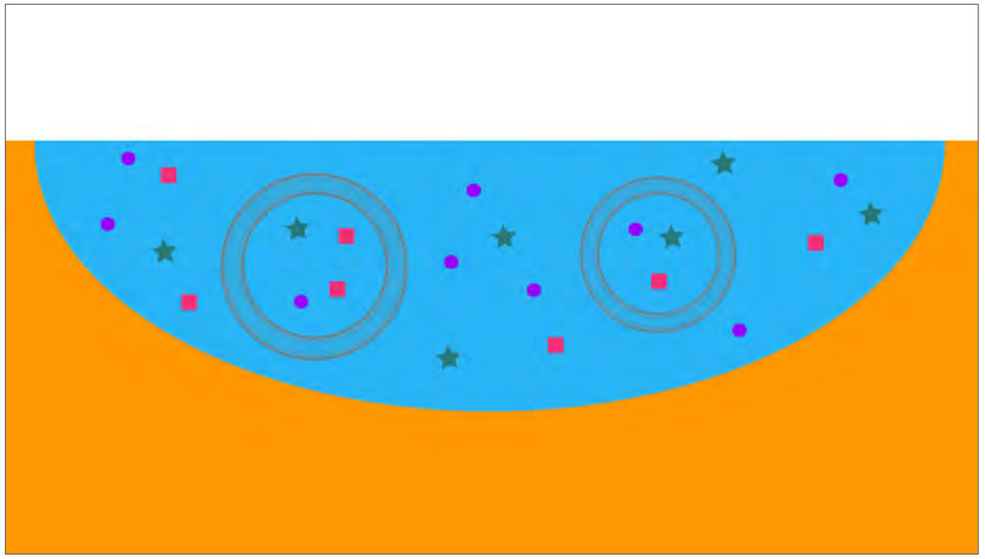

FATTY ACID MEMBRANES ARE STABLE IN CARBONATE-RICH, PREBIOTIC LAKE ENVIRONMENTS

Zachary R. Cohen[1], **Caitlin Cornell[1], David Catling[2], Roy Black[1], Sarah Keller[1]**
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Prebiotic membrane compartments were likely composed of fatty acids. Saturated fatty acids are widely considered to be available in the early Earth environment due to their presence on carbonaceous meteorites[1] and potential abiotic synthesis via Fischer-Tropsch reactions[2]. Here I will show that membrane formation is possible in shallow, carbonate-rich lake environments. These carbonate-rich lakes are attractive sites for prebiotic chemistry for multiple reasons: high carbonate concentrations can help solubilize phosphate minerals[3] and sequester ferrocyanide salts[4], and periodic drying and wetting of shallow water can drive condensation reactions[5]. However, high concentrations of salts have been shown to disrupt formation of pure fatty acid membranes[6]. I have tested mixtures of salts (HCO_3^-, PO_4^-, Cl^- anions) that are likely components of shallow, early Earth lake environments. These experiments show that 2:1 mixtures of decanoic acid and decanol (both putative prebiotic amphiphiles) can form stable compartments in the presence of .5M prebiotic salts. My results strengthen the claim that shallow lake environments are attractive sites for prebiotic chemistry.

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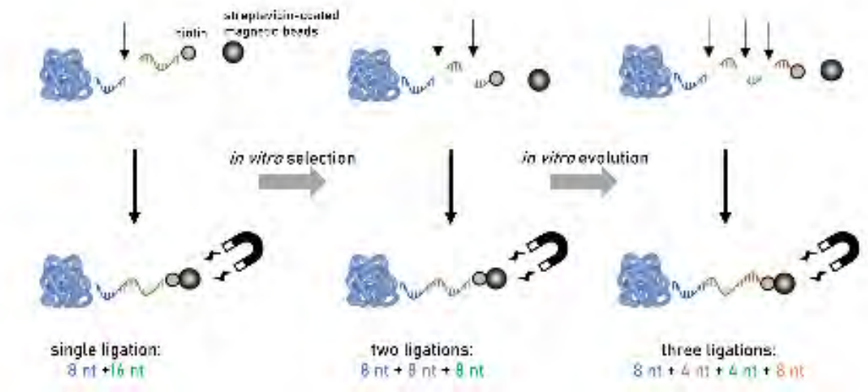
FLOOR 11

Evolving ribozymes to favor ligations of shorter substrates - Short to long RNAs



CHEMISTRY AND CATALYSIS JOIN FORCES IN RNA LIGATION

S.DasGupta[1,2], **T. Walton[1,2], D. Duzdevich[1,2], S.S.Oh[3] and J. W. Szostak[1,2]**
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[2] Department of Genetics, Harvard Medical School,
[3] Pohang University of Science and Technology (POSTECH), South Korea.

The ability of RNA to function as carriers of heritable information and enzymes has made it central to the origin and evolution of life on earth. Since the emergence and advancement of life required propagation of genetic information contained within RNA, in the absence of proteins, we are developing model systems to demonstrate protein-free RNA copying. Non-enzymatic, template-directed polymerization/ligation of intrinsically reactive, potentially prebiotic 2-aminoimidazolide (2AI) monomers/oligomers generate RNA sequences of varying complexity; however, these processes are inefficient[1]. Therefore, the emergence of ribozymes that use these prebiotically-relevant building blocks to assemble complex RNAs more efficiently was perhaps an essential step in the transition from chemistry to biology.
We used in vitro selection to identify ligase ribozymes that utilize 2AI-activated substrates[2]. These ribozymes achieved rate-accelerations of up to 1000-fold. Unfortunately, ligation of short substrates was inefficient. We, therefore, evolved ribozymes that catalyze multiple ligations joining substrates as short as 4 nt long. We also identified ligase ribozymes that function at low Mg^{2+}, making them compatible with vesicular encapsulation by fatty acids. This presents an exciting stride toward achieving compartmentalized RNA-catalyzed RNA synthesis – a major step in the origin of life.

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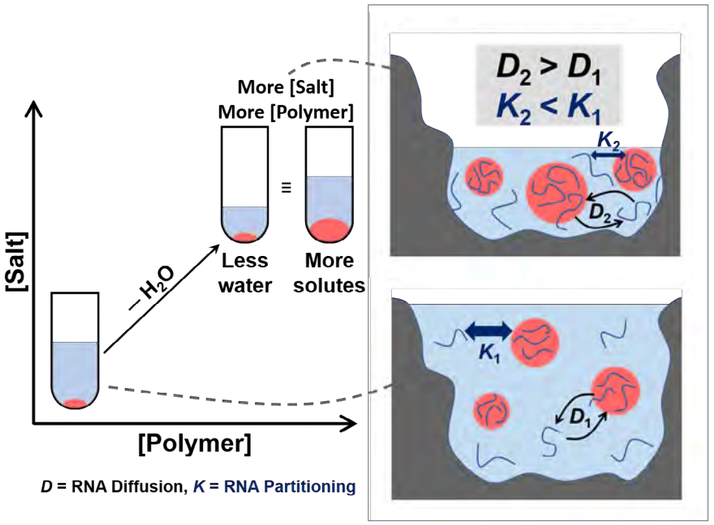

IMPACT OF WET-DRY CYCLING ON THE PHASE & COMPARTMENTALIZATION BEHAVIORS OF COMPLEX COACERVATES

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[2] NASA Postdoctoral Program, Universities Space Research Association, Columbia, MD 21046, USA;
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Wet-dry cycling is an environmental scenario proposed for the increase in molecular complexity on the early Earth. Alternating periods of dehydration-hydration have been shown to promote the production of molecular building blocks of life such as peptides[1] and nucleosides,[2] among others. Studies of the cycle's impact on the assembly of protocells and their functions have been limited. Here, we dehydrated and rehydrated model membraneless compartments made with poly(diallyldimethylammonium)/ poly(acrylic acid). We found that the process led to formation or disassembly of droplets, depending on starting concentrations of the components. The preference of an RNA oligomer to partition within the coacervate phase decreased during tenfold dehydration as its concentration remained constant inside the compartments while increasing tenfold globally. An increase in ionic strength, caused by drying, promoted faster RNA diffusion between the coacervate and its surroundings. After full dehydration, rehydration to the original volume allowed a recapture of original compartments morphology and behavior. Composition mimics, which reproduce the coacervate components concentrations at different steps of dehydration, helped in connecting the drying to linear compositional changes on the coacervate phase diagram. The results emphasize the importance of carefully considering the environment in studies of membraneless coacervate protocells as small alterations can significantly impact their compartmentalization and structural properties.

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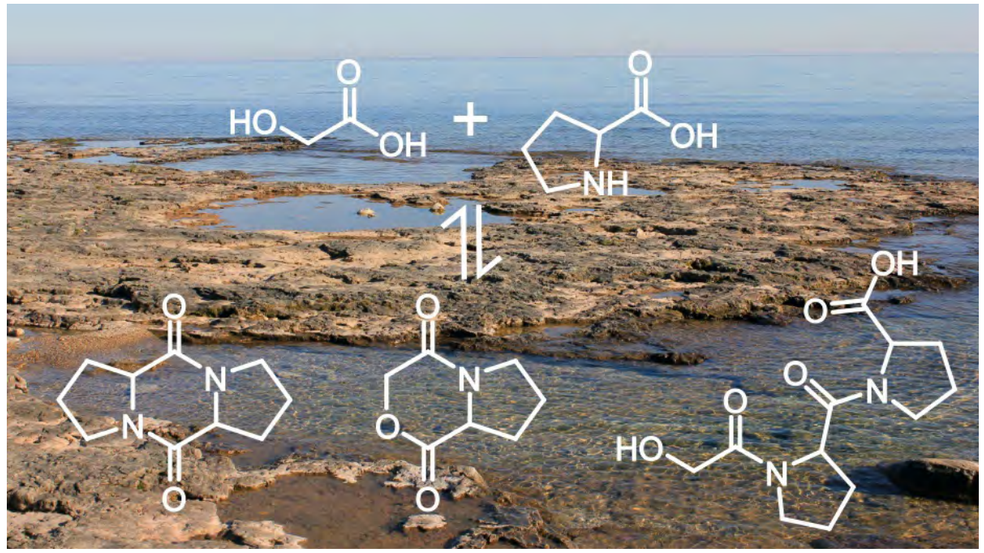

PROLINE INCORPORATION IN MODEL PREBIOTIC DEPSIPEPTIDES

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The chemical evolution of amino acids to peptides with structure and function is of great interest to origins-of-life researchers. Amino acid condensation is unfavorable in water, so various approaches have been explored which polymerize amino acids in model prebiotic scenarios[1,2]. Previously, we demonstrated an approach in which alpha-hydroxy acids condense into oligoesters upon heating and subsequently react with amino acids to form depsipeptides, or amino acid and hydroxy acid copolymers[3,4]. Here, we made mixtures of depsipeptides and compared the incorporation of proline to that of three other prebiotically-plausible amino acids: glycine, alanine, and valine. Oligomers were characterized by mass spectrometry and infrared spectroscopy. Proline was found to incorporate efficiently into linear oligomers, yet it also was detected in small cyclic byproducts. Proline is known to induce unique structural properties in biological peptides and warrants further study in the context of proto-peptide evolution.

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NUCLEOTIDE-LEVEL RESOLUTION OF RNA FOLDING INTERACTIONS WITHIN PEPTIDE-BASED COMPLEX COACERVATES

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The RNA World Hypothesis states that RNA or an RNA-like polymer may have acted as both the initial genetic material and the catalyst for the reactions of life. In the 1980s, the first ribozymes were discovered, demonstrating that RNA could act as a catalyst. Since then, it has become apparent that RNA folding is integral to function in a way similar to protein enzyme folding. Because of this, it is important to try to understand RNA folding under prebiotically relevant conditions.
On the early Earth, a problem that would have been faced by the first enzymes was the scarcity of organic material. To overcome this issue, organic material would need to be localized and concentrated on either a mineral surface or in some type of compartment, like a protocell.
An ideal protocell candidate should partition molecules required for catalysis such as: Mg^{2+}, nucleotides, RNAs, amino acids, and peptides. A model protocell that is able to do this is complex coacervates.
Herein, I describe RNA folding studies within complex coacervate droplets made out of Lys_n-Asp_n, and Lys_n-ATP. A model functional RNA with a well-defined three-dimensional structure, $tRNA^{phe}$ from *S. cerevisiae*, was used for these initial RNA folding studies. $tRNA^{phe}$ was subjected to in-line probing (ILP) under the following conditions (0.5 mM Mg^{2+}, 15 mM KCl, and 10 mM Tris, pH 8.3) initially to determine its native fold. Then, $tRNA^{phe}$ was placed inside of Lys_n-Asp_n and Lys_{10}-ATP coacervates where we found that under all of these coacervate conditions, the tRNA had lost its tertiary contacts and the acceptor stem was unfolded. Upon changing Mg^{2+} conditions and charge-ratio of polyanions to polycations, more native folding of $tRNA^{phe}$ was observed. Future studies will focus on evaluating if similar trends will be seen for ribozymes under the above conditions.

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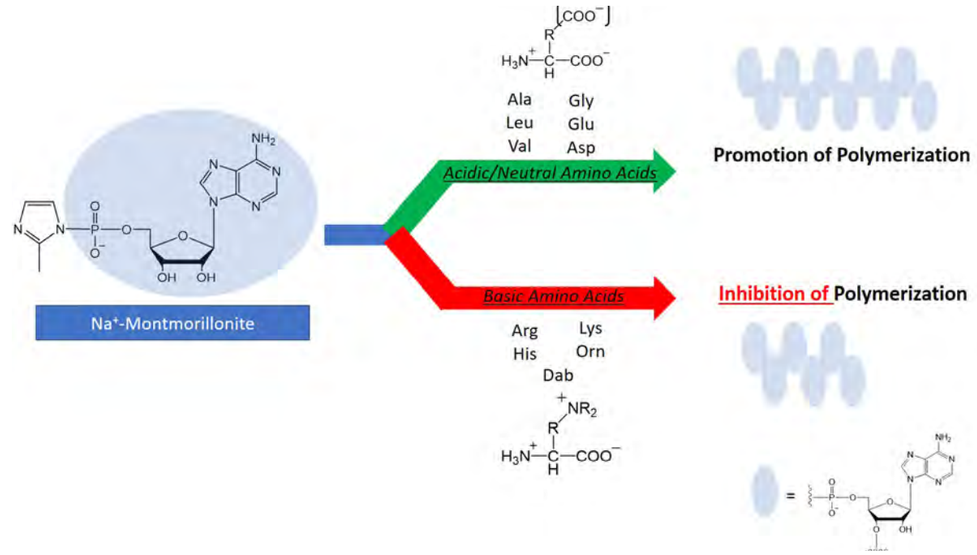

ROLE OF AMINO ACIDS ON NONENZYMATIC CLAY-PROMOTED OLIGOMERIZATION OF ACTIVATED NUCLEOTIDE

Trishool Namani[1], Savannah Snyder[2], James Eagan[1], Philip C. Bevilacqua[3], Chrys Wesdemiotis[2], and Nita Sahai[1]
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RNA biopolymer synthesis from prebiotically possible molecules is one of the important steps in the early evolution of life on Earth, hence numerous studies have reported on oligonucleotide synthesis under various experimental conditions[1,2]. Montmorillonite clay was extensively studied as a reaction promoter for activated nucleotides forming RNA polymer[1,3]. In the present study, we have examined a multicomponent system in which amino acid and montmorillonite clay both influence the polymerization of activated mononucleotide, adenosine 5'-phospho-2-methylimidazolide (2-MeImPA) polymerization at neutral pH. The polymerization of 2-MeImPA is further promoted in the presence of acidic and neutral nonpolar amino acids, which results in longer oligomers than the clay system alone. Positively charged amino acids, by comparison, exhibit an inhibitory effect and create shorter oligomers. To understand the impact of amino acids on 2-MeImPA polymerization, we hypothesize: 1) the acidic and non-polar amino acids are anchored to the negatively charged clay surface sites through their alpha ammonium group, while the alpha carboxylate interacts with the methylimidazolium ring of the activated nucleotide providing an ideal conformation to convert the activated nucleotide into a better leaving group, thus creating longer oligomers, 2) the basic amino acids bind with their basic side chain to the montmorillonite surface and compete with the mononucleotide for adsorption to the clay surface, thus resulting in shortened oligomers.

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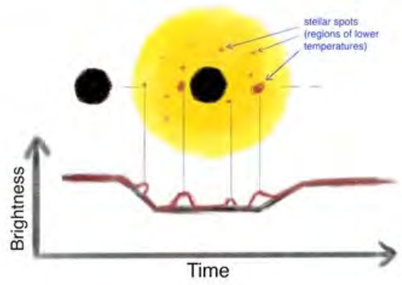
Using Machine Learning to Improve Prediction of Chemical Composition of Exoplanetary Atmospheres



USING MACHINE LEARNING TO IMPROVE PREDICTION OF CHEMICAL COMPOSITION OF EXOPLANETARY ATMOSPHERES

Artash Nath
Co-founder, HotPopRobot.com

Humankind does not currently possess instruments to detect life on exoplanets – planets outside the solar system. But efforts are ongoing to come up with newer ground and space-based telescopes that could help us learn more about atmos-pheres of these exoplanets.
When an exoplanet transits in front of its parent star, its main body blocks out some light of the star. This causes a dip in the light received from the star. If the exoplanet has an atmosphere around it, then the atmosphere will also absorb some of this light. How much light is absorbed by the atmosphere depends on its thickness and gases present.
Different gases absorb different wavelengths of light to different degrees. If we plot the transit of an exoplanet in different wavelengths, we will get light curves of different depths. Studying transit light curves of exoplanets in different wave-lengths could help us predict the chemical composition of their atmospheres.
However, the parent star of the exoplanet may have stellar spots that are cooler than the surrounding surface. This adds noise in the data. We must isolate depth in light curves caused by the exoplanetary atmosphere from those caused by the stellar spots. The current approach is to remove this noise manually which is time consuming and prone to errors.
Applying machine learning to exoplanetary data may help remove the noise of star-spots in data on transiting exoplanets' atmospheres received by space tele-scopes. I created a Hybrid Machine Learning model using Long-Short Term Memory (LSTM) - a form of Recurrent Neural Network (RNN) to reduce this noise. My model was able to accurately predict the exoplanet-star radius ratio in 55 wavelengths with a mean square error of 0.001. The Algorithm leads to elimination of noise and may lead to improved and accu-rate prediction of chemical composition of exoplanetary atmospheres.

The simulated dataset I used for my project can be accessed from the ARIEL Space Telescope Machine Learning Challenge website at: https://ariel-datachallenge.azurewebsites.net/ML

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EXOPLANETARY ATMOSPHERIC RETRIEVAL USING MACHINE LEARNING

Aline Novais[1], Luan Ghezzi[1], Kevin Heng[2]
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[2] Center for Space and Habitability, University of Bern, Switzerland

Although the analysis of exoplanet atmospheres has become one of the most pertinent topics within planetary science, characterizing these objects directly from their spectra might still be a challenge. To interpret the spectrum of an exo-atmosphere, one can apply an inverse technique known as atmospheric retrieval, which is the use of an observed transmission spectrum to infer planetary properties, such as its temperature profile, chemical composition and atmospheric circulation. This work establishes if the stellar radius' and gravity of the exoplanet's uncertainties cause non-negligible effects in currently available HST Wide Field Camera 3 (WFC3) and Space Telescope Imaging Spectrograph (STIS) spectra and in future spectra measured by JWST. We intend to determine when the effects of critical spectral resolution and wavelength coverage are important, so as to guide future procurement of exo-atmospheric spectra. Consequently, we will establish the conditions under which the analytical formula for isothermal, isobaric transit chords breaks down and a full numerical treatment is needed instead.

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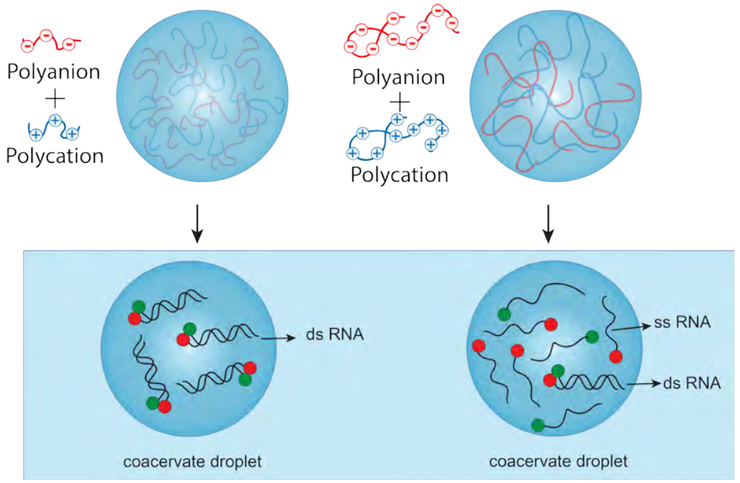

PREBIOTICALLY-RELEVANT LOW POLYION MULTIVALENCY MIGHT IMPROVE FUNCTIONALITY OF MEMBRANELESS COMPARTMENTS

Fatma Pir Cakmak[1], **Saehyun Choi[1], McCauley O. Meyer[2,3], Philip C. Bevilacqua[1,2,3] and Christine D. Keating[1]**

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Multivalent polyions can undergo complex coacervation, producing membraneless compartments that accumulate ribozymes and enhance catalysis, and offering a mechanism for functional prebiotic compartmentalization in the origins of life. Here, we evaluated the impact of low, prebiotically-relevant polyion multivalency in coacervate performance as functional compartments. As model polyions, we used positively and negatively charged homopeptides with one to 100 residues, and adenosine mono-, di-, and triphosphate nucleotides. Polycation/polyanion pairs were tested for coacervation, and resulting membraneless compartments were analyzed for salt resistance, ability to provide a distinct internal microenvironment (apparent local pH, RNA partitioning), and effect on RNA structure formation. We find that coacervates formed by phase separation of the relatively shorter polyions more effectively generated distinct pH microenvironments, accumulated RNA, and preserved duplexes. Hence, reduced multivalency polyions are not only viable as functional compartments for prebiotic chemistries, but they can offer advantages over higher molecular weight analogues.

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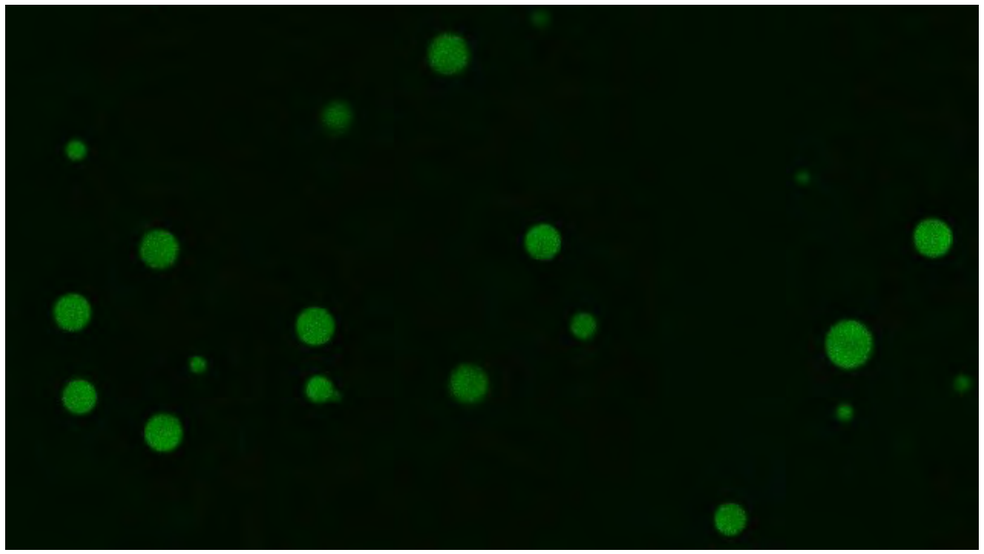

RNA WORLD INSIDE COMPARTMENTS: ACTIVATION OF RNA CATALYSIS BY COMPLEX COACERVATES

Raghav R. Poudyal[1], **Rebecca M. Guth-Metzler[3*], Andrew J. Veenis[1], Erica A. Frankel[1#], Christine D. Keating[1,2], Philip C. Bevilacqua[1,2,3]**

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Complex coacervates are non-membranous compartments (NMCs) formed by associative phase separation of oppositely-charged polyelectrolytes. Owing to their ability to encapsulate biomolecules, they have been postulated as alternative prebiotic compartments. In this study, we report that NMCs of complex coacervates can concentrate RNA oligonucleotides and activate catalysis of multiple nucleic acid enzymes, including a deoxyribozyme. Furthermore, we reveal that polyanions can tune microenvironments of NMCs to further enhance RNA catalysis. By competing for unproductive RNA- polycation interactions, short polyanions enhance ribozyme reactions more than 12-fold. Productive RNA interactions in NMCs that are otherwise inaccessible in dilute solutions reveal potential roles for these compartments in the context of origin of life and extant biological intracellular condensates.

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DEFINING LYFE IN THE UNIVERSE: FROM THREE PRIVILEGED FUNCTIONS TO FOUR PILLARS

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Motivated by the need to paint a more general picture of what life is—and could be—with respect to the rest of the phenomena of the universe, we propose a new vocabulary for astrobiological research. Lyfe is defined as any system that fulfills all four processes of the living state, namely: dissipation, autocatalysis, homeostasis, and learning (see Figure)[1]. Life is defined as the instance of lyfe that we are familiar with on Earth, one that uses a specific organometallic molecular toolbox to record information about its environment and achieve dynamical order by dissipating certain planetary disequilibria. This new classification system allows the astrobiological community to more clearly define the questions that propel their research—e.g., whether they are developing a historical narrative to explain the origin of life (on Earth), or a universal narrative for the emergence of lyfe, or whether they are seeking signs of life specifically, or lyfe at large across the universe. While the concept of "life as we don't know it" is not new, the four pillars of lyfe offer a novel perspective on the living state that is indifferent to the particular components that might produce it.

1 Bartlett, S and Wong, M L (accepted) Defining Lyfe in the Universe: From Three Privileged Functions to Four Pillars, Life

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DECIPHERING NONENZYMATIC RNA POLYMERIZATION THROUGH CRYSTALLOGRAPHY

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Many high resolution crystal structures have contributed to our understanding of the reaction pathway for catalysis by DNA and RNA polymerases, but the structural basis of nonenzymatic template-directed RNA replication has not been studied in comparable detail. Here we present crystallographic studies of the binding of ribonucleotide monomers to RNA primer-template complexes, with the goal of improving our understanding of the mechanism of nonenzymatic RNA copying. Using our synthetic unreactive phosphonate-linked analog of activated monomer, we obtained the structures of RNA primer-template complexes with the monomers bound. Our structures demonstrate the versatile binding motifs of activated mononucleotide substrate in nonenzymatic RNA polymerization, which could significantly influence the rate and fidelity of RNA replication, and they also illustrate the structural rationale of the great catalytic function of the downstream helpers. In addition, our time-resolved structures successfully integrate several static RNA-substrate structures into a molecular "movie" following the reaction process, and it clearly reveals the mechanism of RNA nonenzymatic replication. Against the traditional opinion that the catalysis of downstream activation is based on the noncovalent leaving group-leaving group effect, our time-resolved structures demonstrate that the facilitation is from the formation of imidazolium-bridged intermediate. Our structures provide the powerful tool and fundamental evidence for the RNA self-replication mechanistic studies.

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COMPUTATIONAL STUDY OF PHYSICOCHEMICAL PROPERTIES OF AN ADENINE SYNTHESIS ROUTE UNDER UV RADIATION

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One of the most important topics of the origin of life studies is the searchfor plausible routes of prebiotic synthesis of fundamental molecules for living beings. Since the experiments carried out by Miller up to date, many environments have been simulated for the conditions of the Earth 3.8 Ga ago. They have managed to synthesize nucleotides, amino acids, among other essential components for life. All these studies have found that in order to trigger the synthesis reactions of molecules of prebiotic importance, it is necessary to supply some type of energy such as temperature, electric discharges, radiation, etc(Barks etal. 2010)). The surface of the Earth during the Archean period (approximately 3.8 Ga) was exposed to higher doses of UVC radiation (200-280 nm) and UVB (280-315 nm) in comparison with the radiation that arrives to the Earth today (Sagan, 1973; Cockell, 1998). The reason for thishigh UV irradiation was thelack of layer of ozone and higher emissionof the Sun in this wavelength range.In this sense, UV radiation might have played animportant role in the evolution of prebiotic chemistry. In an astrobiological context, all stars emit UV radiation;particularly dwarf M-type stars (Hunt-Walker et al., 2012). TheUV flux on a planetary surface of a potentially habitable hypothetical planetdependson itsatmospheric composition and the spectral type of the hosting star. This fact might thus change the potential chemical reactivity and synthesis of some organic compounds on the planet (Rugheimer et al., 2015). For our work we analyzeda known route of adenine prebiotic synthesis from formamide using the HyperChem software.We analyzed some physicochemical properties (oscillator strength, energy difference between the HOMO-LUMO orbitals and dipolar moment among others) of intermediate molecules in this path under the interaction with an UV photon.Here, we present the preliminary results on how UV radiation affects these molecules of prebiotic importance and the possible triggering effect of UV radiation to promote physicochemical reactions for its production.

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ENDOLITHIC CULTURABLE BACTERIA IN MINERALS (QUARTZ, K-FELDESPAR, CALCITE) FROM GEOLOGIC SAMPLING IN VILLA DE LEYVA, BOYACA & PESCADERO, SANTANDER (COLOMBIA)

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Endolithic microbial communities have been reported in arid and hyperarid zones around the world. Also, it has been found that bacteria use as microhabitat different lithologies, whose chemical elements may act as a nutritional source. This study focuses on the relation between culturable endolithic microbes and three rock-forming minerals (quartz, k-feldspar and calcite) in order to determine the potential of these minerals to serve both as a microhabitat and as a source of nutrients. Geological data collected in two localities in Colombia: Villa de Leyva, Boyacá (5°36′ 24.12″ N, 73° 31′ 31.32″ W) and Aratoca, Santander (6°49′ 0.62″ N, 73°0′ 20.3″ W) along with microbiological data obtained in the laboratory provide information about the affinity between native endolithic microbial communities and the three mentioned minerals. In order to determine geochemical characteristics of the minerals X-Ray Fluorescence (XRF), environmental scanning electron microscopy (ESEM), and Petrographic analysis were carried out. Additionally, microbiological procedures [culture techniques, gram stain and physicochemical profile] were performed to characterize the colonies of native endolithic culturable microorganisms along with climatological data from the study areas. Multiple Correspondence Analysis (MCA) was used to discover whether there are relationships between microbes and some abiotic conditions. In this study we discuss that rock-forming minerals calcite, K-feldspar and quartz act as a potential microhabitat for microbes and that its bio-receptivity could be useful for the search of extraterrestrial life on Mars surface.

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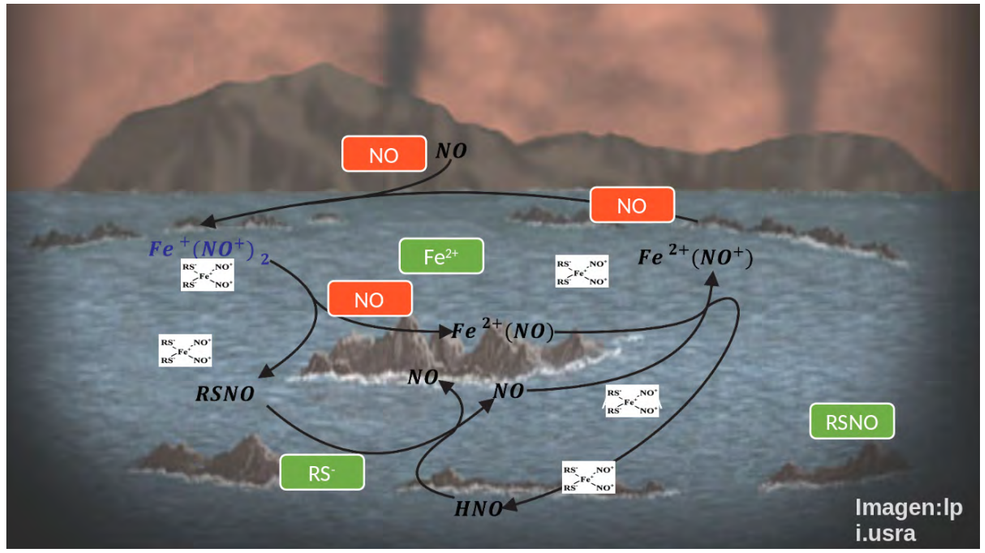

CHEMICAL OSCILLATIONS IN A THEORETICAL SYSTEM OF DINITROSYL IRON COMPLEX (DNIC) WITH THIOL-CONTAINING LIGANDS

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Anatoly Vanin and his research group have been involved for more than 50 years in an extensive study on the preponderant role of the iron dinitrosil complexes (DNICs) in biological systems. Owing to its simple structures, it constitutes a work-ing form of endogenous nitric oxide in alive systems. The involvement of nitric oxide as a universal regulator present in all known life forms led to the important conclusion regarding the leading role of that have played the DNICs both at the present and in the past in the definition of the metabolic processes of living be-ings. Ferrous ion and nitrosothiols are the building blocks through an enriched chemistry stand out over other regulatory mechanisms. Vanin's reaction be-tween the ferrous ion and nitrosothiols have shown attenuated fluctuations in the DNIC concentration in a time interval of 500 to 2500 s. Considering the high pos-sibility of real oscillations in the Vanin's work, the present study has reanalyzed the kinetic model proposed by Dr. Vanin in his original work[1] and investigated other possible mechanisms linking the traditional Vanin model with chemical os-cillations. The simplicity of this mechanism, and the possibility that it does not involve advanced biochemical species such as enzymes, allow us to infer that it is very likely that this is a mechanism of temporal-spatial regulation[2] is very old and associated with each domain of life, even early life[3]. As Epstein has indicated[4] if the experiments and the mechanism agree, we can maintain the mechanism and try some more experiments; for this reason, this work seeks to motivate to continue investigating experimentally the oscillations that can oc-cur in this type of systems that Vanin has studied.

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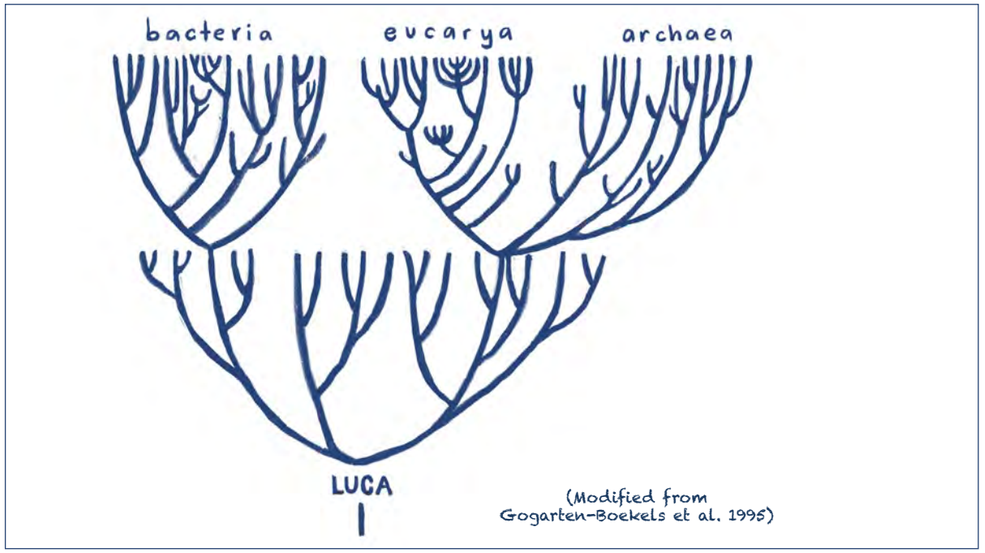

WAS LUCA A HYPERTHERMOPHILIC PROKARYOTE? THE IMPACT-BOTTLENECK HYPOTHESIS REVISITED

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In the Origin of Species, Darwin wrote "The affinities of all the beings of the same class have sometimes been represented by a great tree. I believe this simile largely speaks the truth." Modern comparative genomics has revealed that the intuition of Darwin was correct. A set of highly conserved genes and cellular functions indicate that all life on Earth is related by common ancestry. These genes were inherited from the Last Universal Common Ancestor or LUCA. The functions coded by these genes suggest that LUCA was a rather complex cell already endowed with a genetic code and a protein translation apparatus. One of the questions regarding the nature of LUCA is whether it was a hyperthermophile. Here, we review recent evidence derived from the molecular fossil record on the temperature preferences of LUCA. We suggest that current evidence on the nature of LUCA and its immediate predecessors are compatible with the impact-bottleneck hypothesis – the proposal that during the early evolution of life a meteoritic impact eliminated all life on Earth except for prokaryotes capable of living at high temperatures. If our interpretation of the data is correct, it would indicate that early life was resilient to the rough environmental conditions of the Archean. A relevant result from the point of view of astrobiology because it would exemplify the persistence of life in harsh environments.

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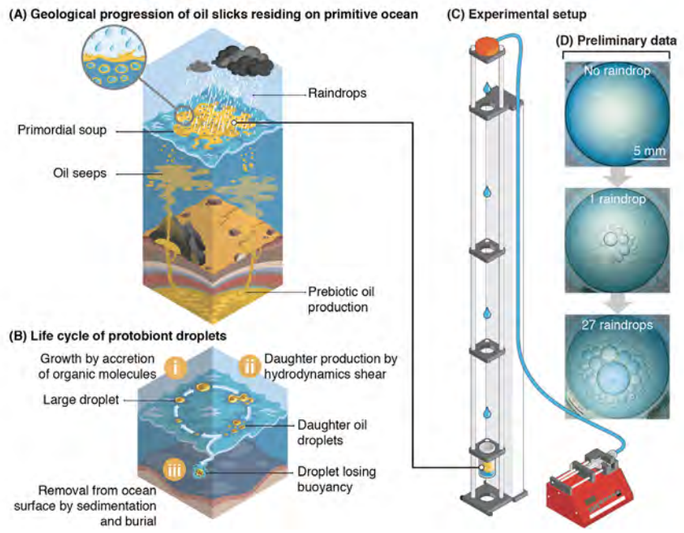

Fig. 1. Raindrop impacting prebiotic soup of oil film residing on ocean water produces protocell "droplets".
(A) Schematic of proposed geological progression of oil slick production on primitive ocean followed by action from raindrop impact forming oil droplets and cell-like structure droplets.
(B) Life cycle of the proposed protobionts of oil droplets.
(C) Experimental setup to generate raindrop impacting on oil film residing on ocean water.
(D) Preliminary data of droplet formation at indicated raindrop numbers.

PRODUCING CELL-LIKE STRUCTURES FROM OIL FILMS RESIDING ON OCEAN WATER BY RAINDROP IMPACTS

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Progress in the bottom-up construction of synthetic cells[1] has given insights into how biological organisms function and on the origins of life. Despite advances in the last decades, a demonstration of an open-ended in-vitro evolution of synthetic cells that is simple enough to serve as a plausible model of the prebiotic/biotic transition has yet to be demonstrated. Here, we develop a synthetic cell platform based on geophysical considerations. We model the protocell as oil-inwater droplets. While there have been several works demonstrating oil-in-water droplets exhibiting the behaviors that protocell may encounter,[2,3] there have yet a complete demonstration of oil-in-water droplet that can undergo a complete life cycle involving birth, growth, replication, and death, within a plausibly prebiotic environment. The proposed model centers on the ubiquitous mechanical processes in the dispersal of natural and manmade oil slicks in modern oceans. In the prebiotic world, the organic matter, primarily delivered to the earth's surface by micrometeorites, would have naturally accumulated to ocean surface as oil slicks.[4] Additionally, these organic compounds were, perhaps, prevented from reaching shore by entrapment in ocean gyres. Hydrodynamics forces such as raindrops or breaking waves on these thick organic films, resembling a primordial soup, would have produced droplets (Fig. 1A). Similar notion was proposed by Oparin where hydrodynamic forces play an important role on the origins of life by enabling Darwinian evolution in the fragmentation of coacervates through hydrodynamic shear.[5] Comparably, the oil droplets could have undergone growth via accumulation of organic compounds (Fig. 1B–i), fission via locally intense hydrodynamic shear produced by rainfall or breaking waves (Fig. 1B–ii), and eventually death by burial via the loss of buoyancy through mineral accumulation (Fig. 1B–iii). In short, these droplets could have functioned as simple self-replicators that natural selection could act to select droplets possessing more fit chemical and structural composition, and ultimately giving rise to the protobionts. Finally, we will present results from preliminary laboratory experiments that explore the rich fluid-mechanics phenomena involved in the production of oil droplets from hydrodynamics forces acting on oil films residing on water surfaces and in the fissioning of oil droplets (Fig.

1C). In particular, raindrop impacting oil film residing on water also produces water-in-oil-in-water (w/o/w) droplets that resemble lipid vesicles in that a volume of water is surrounded by film of oil (Fig. 1D). Such droplets may have facilitated the prebiotic/biotic transition. Stability test reveals that the droplets can maintain its identity up to three days if PEG-octyl-ether is used as the surfactant. In contrast, the droplets are only stable on a time scale of minutes for PEG600-cholesterol surfactant.
Further experimental development may lead to a bench-top system in which oil droplets undergo growth and fission, and are maintained at a steady state concentration through continual removal of oil droplets which is analogous to a death process in natural environment. The population of oil droplets maintained by such a system could serve as a platform for in-vitro evolution.

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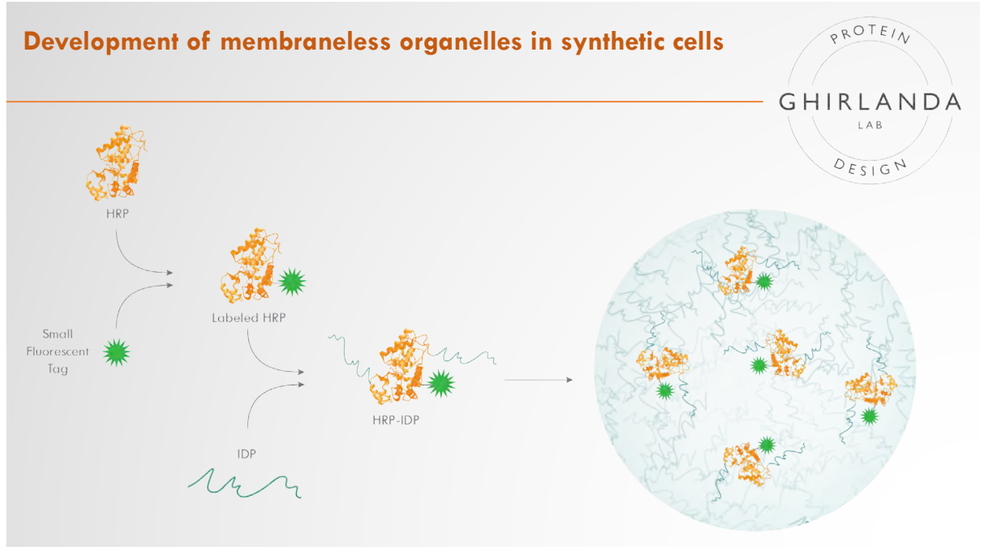

MEMBRANELESS ORGANELLES BY DESIGN

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Compartmentalization is at the basis of cellular organization. Traditional organelles are delineated from the cytoplasm with a semi-permeable lipid bilayer and are considered permanent structures. In addition, cells comprise functional membraneless organelles such as the Cajal body and the nucleolus, in both the nucleus and the cytoplasm, that contain high concentrations of proteins. It has been recently established that these structures form by liquid liquid phase separation of nucleic acids and/or proteins, and carry out diverse functions in the cell. They form and disperse in response to the cellular environment and, without a membrane, are accessible to the surroundings through equilibrium.
Our group is designing functional membraneless organelles formed by liquid-liquid phase separation as compartments for synthetic cells. Here, we use fused in sarcoma (FUS) and a DEAD-box helicase (Ddx4), which form LLPS droplets in certain conditions, as elements to drive the localization of enzymes into an artificial organelle. Specifically, the sequences corresponding to wild-type FUS (residues 1-214, from here on defined as N-FUS), and to wild-type Ddx4 (residues 1-236, N-Ddx4), were conjugated to horseradish peroxidase. The phase diagram describing the spinodal and binodal transition to form LLPS droplets is experimentally determined by DLS, both before and after conjugation. Fluorescent microscopy was used to confirm the presence of conjugated enzymes within the concentrated droplets. We are currently investigating the activity of enzymes within the droplets. Finally we will test the effectiveness of LLPS droplets in organizing and enhancing the activity of enzymatic cascades, starting with two well-known model systems: the two-enzyme GOx/HRP system, and the more challenging three enzyme cascade that forms the methanol dehydrogenase pathway (ADH/ALDH/FDH). Future work will address the enzymatic efficiency of the system through absorbance of the final product in kinetic assays.

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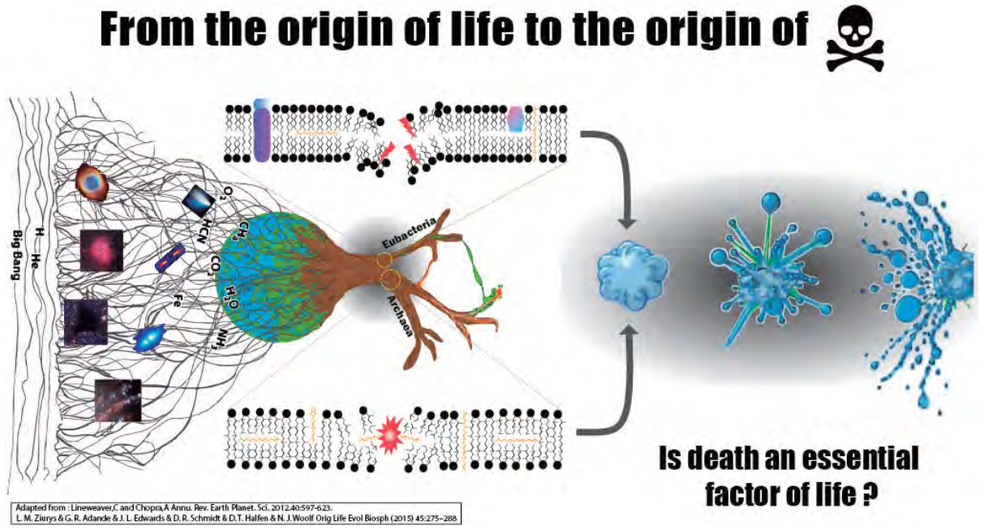

WHAT ABOUT THE ORIGIN OF DEATH?

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The emergence of life implies the origin of an archaic form of death. From our understanding of primitive cells, the death state must have been based on thermodynamic/material starvation[1], a phenomenon understood as the irreversible transition of a system from the dynamic kinetic stability status, of the replicative world, to the thermodynamic world[2].

The adaptative responses that early life set towards different agents that compromise cell vitality, such as: temperature shock, oxidative stress, DNA damage, and pathogens, constituted the evolutionary origin of senescence[3]. Nowadays, when modern prokaryotic cells accumulate endogenous damage, they enter a non-proliferating state ruled by many molecular alterations that could have been established during the conformation of LUCA[4].

Additionally, collapse and depolarization of the membrane generates a decline in the ATP levels and the release of free radicals, a classic sequence that triggers programmed cell death[5]. However, LUCA's membrane type, respiratory complexes and ATP-synthase status remains a subject of discussion between two main approaches for life's site of origin: the sub-areal hot springs and the hydrothermal vent hypothesis. Environmental conditions on these sites, proton permeability, and membrane antiporters nature would have evolved different properties, implying distinct responses to agents that may cause the first death of a living cell.

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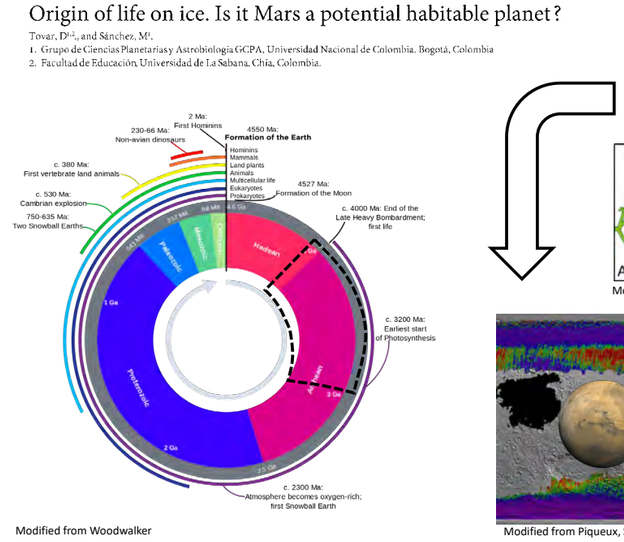

ORIGIN OF LIFE ON ICE. IS MARS A POTENTIAL HABITABLE PLANET?

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Broad consensus among scientific community on the origin of life on Earth, suggests that it may have originated from hydrothermal underwater vents at temperatures close to 250 ° C[1]. However, low concentration of greenhouse gases such as CO2 and water vapor in the Archean, contribute to ubiquitous frozen oceans[2,3].

Frozen oceans are usually associated in most cases with Earth´s poles. An atmosphere generated by degassing due to asteroid impacts instead of continuous degassing, indicates that the presence of greenhouse gases is low at the primitive Earth[2,3]. During the Archaean, the relationship between the rate of microbial metabolism in ice and the rate of experimentally determined production of trapped gases of microbial origin, might explain the rate of methane production as a function of temperature from their habitat. This could be applied even on Mars currently[4,5].

These reactions exhibit geophysical and geochemical characteristics that can be found at very low temperatures, since the interface of prebiotic activity with icy terrestrial environments is a dynamic environment where these microbes have been found to eventually thrive[2,5].

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EXTREMOPHILIC PROTEINS AND THEIR RESISTANCE SECRETS

Alfredo Rodríguez Arteaga
Institute of Biotechnology of the UNAM, Mexico

All the cells of all the organisms we know have proteins that function as molecular factories to make copies of their genetic material and, of course, have ways to repair it from almost any damage they are exposed to on earth. Like the cases of extremophiles that survive in places where we cannot. The proteins of the extremophiles reveal to us their peculiarities and potential of applications. In this project I will talk about the use of X radiation to extract the secrets of a protein involved in the replication and repair of DNA from all terrestrial organisms. Its name is Nuclear Antigen of Proliferating Cells or PCNA for short. This protein has no enzymatic activity but plays the role of a sliding clamp. Enzymes from different families and functions such as DNA Ligase or DNA Polymerase are attached to PCNA.

The reasons that amaze us about this protein was that when irradiating the PCNA of Thermococcus gammatolerans with X-rays, it did not suffer any of the usual damages observed in other proteins.

We bioinformatically explore the three-dimensional structure of this PCNA and analyze it evolutionarily. In other words, we explore their possible changes over time. Now we have a set of secrets that we steal from these proteins about their resistance. We are amazed at the results because they have enormous application potential to modify molecules of other organisms that cannot resist radiation but are indispensable in our daily lives, especially microorganisms. This represents a contribution to the nascent field of Synthetic Astrobiology that is the combination of modified organisms in the laboratory with there applications to astrobiology. Our dream for the future is the usage of this information to modify important organisms so that they survive extraterrestrial conditions and help our travel trough the stars.

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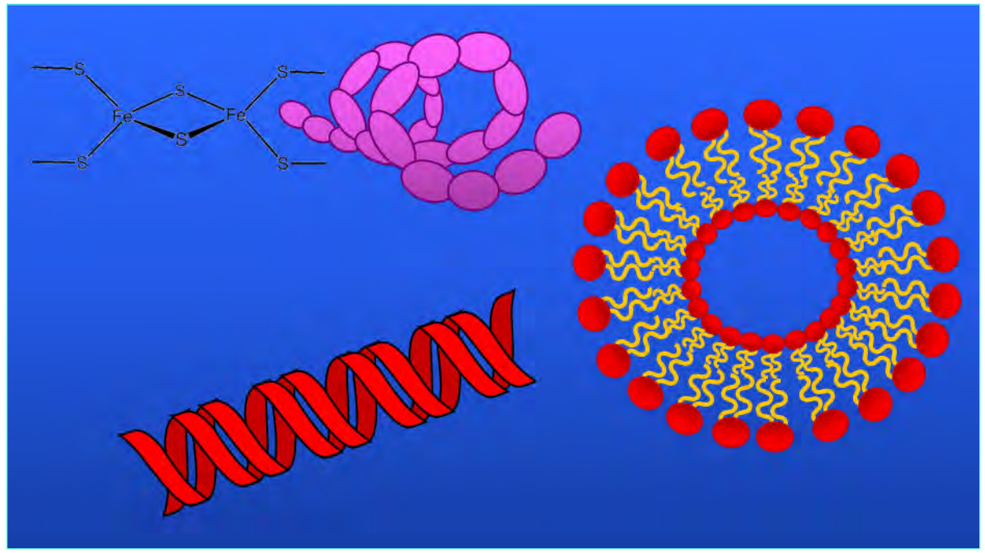

CONTRAST BETWEEN THE MAIN LIFE'S ORIGINS ABIOGENIC MODELS

Rodríguez-Torres, L. M., Quintero-Luis, R., Carreño-López, R.
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Currently, theories have been developed that seek to explain the origin of life from abiogenesis, however there are so many theories that they can be grouped into models. The 'genetics-first' model has the most accepted theory: RNA world, this molecule has important properties but it is too labile. Besides, the 'metabolism-first' model has a theory that has acquired importance: Iron-sulfur world, the energy released from the metal sulfides was available for the synthesis of organic molecules and the formation of polymers. Finally, the 'co-evolution of the three components' model takes some elements of the theories presented previously to generate a more complete and solid explanation but it has only one theory, which is based on peptide/oligonucleotide interdependence in relation with oil slick. This review contrasts these models and suggests the need to test them by well-designed experiments.

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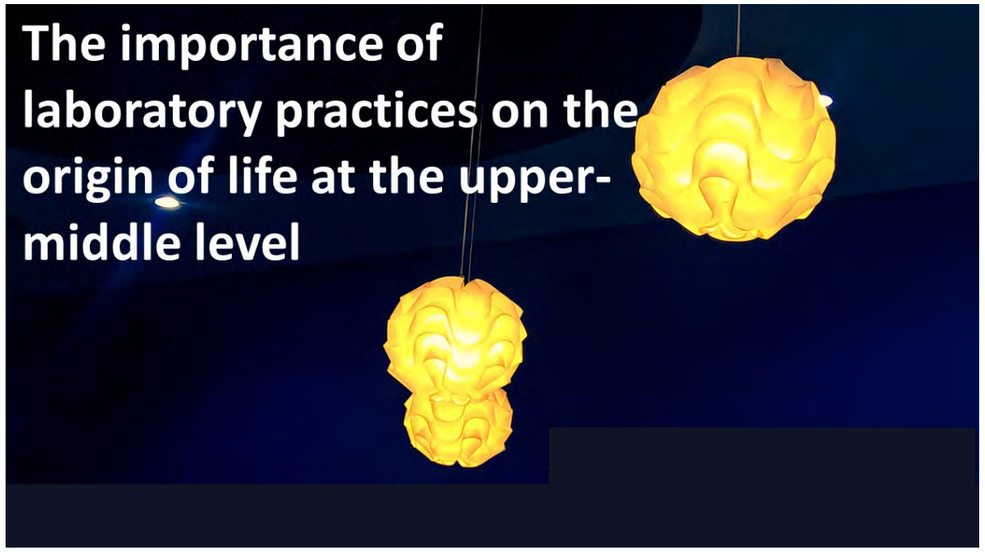

THE IMPORTANCE OF LABORATORY PRACTICES ON THE ORIGIN OF LIFE AT THE UPPER-MIDDLE LEVEL

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The society in which the human being operates at present is a society characterized mainly by great scientific and technological advances and above all by the great dependence on technological devices, however, scientific illiteracy is just as broad, it is, therefore, from the schools, this scientific and technological knowledge of individuals at all educational levels must be worked on and struc-tured. In the school system corresponding to the upper secondary level in Mexico, there is a great diversity of subsystems which aim to satisfy the demand and coverage of the population in terms of access to education. Said subsystems approach biology in a similar way where the curriculum focuses mainly on systems theory with an emphasis on ecology and the environment, on average they take 3 to 5 hours/week/month, which leaves little time to deal with other topics of biological importance, this research aims to analyze how the topic of the Origin of Life is addressed as well as the laboratory practices that are implemented to reinforce the topic. Seven higher-level educational subsystems contained in four public educational systems were analyzed, which were:

Public Educational System	Subsystem
National Autonomous Uni. of Mexico (UNAM)	College of Science and Humanities (CCH)
	National High School (ENP)
National Polytechnic Institute (IPN)	Centers for Scientific and Technological Studies (CECyTs)
Undersecretary of Higher Middle Edu. (SEMS)	National College of Technical Professional Education (CONALEP)
Institute of Higher Middle Education (IEMS)	College of Baccalaureates (COLBACH)
	Directorate-General for Baccalaureates (DGB
	Mexico City High Schools

The results show that the topic of the Origin of life is approached in a theoretical way and some subsystems it does not exist in its study plan or it is approached superficially emphasizing the theoretical part where students are invited to de-bate the different theories of the origin of life integrating the social and cultural aspects of the historical moment when the theory was raised, in some subsys-tems a timeline of theories of the origin of life is requested. Regarding the labora-tory sessions, it was found that the experiment to be carried out is that of Francis-co Redi and the meat in jars. However, the results obtained by the students con-fuse them depending on the type of meat they use. Another practice found was the formation of coacervates with grenetine which interested the students, how-ever, the use of microscopes is necessary and some subsystems lack this re-source.

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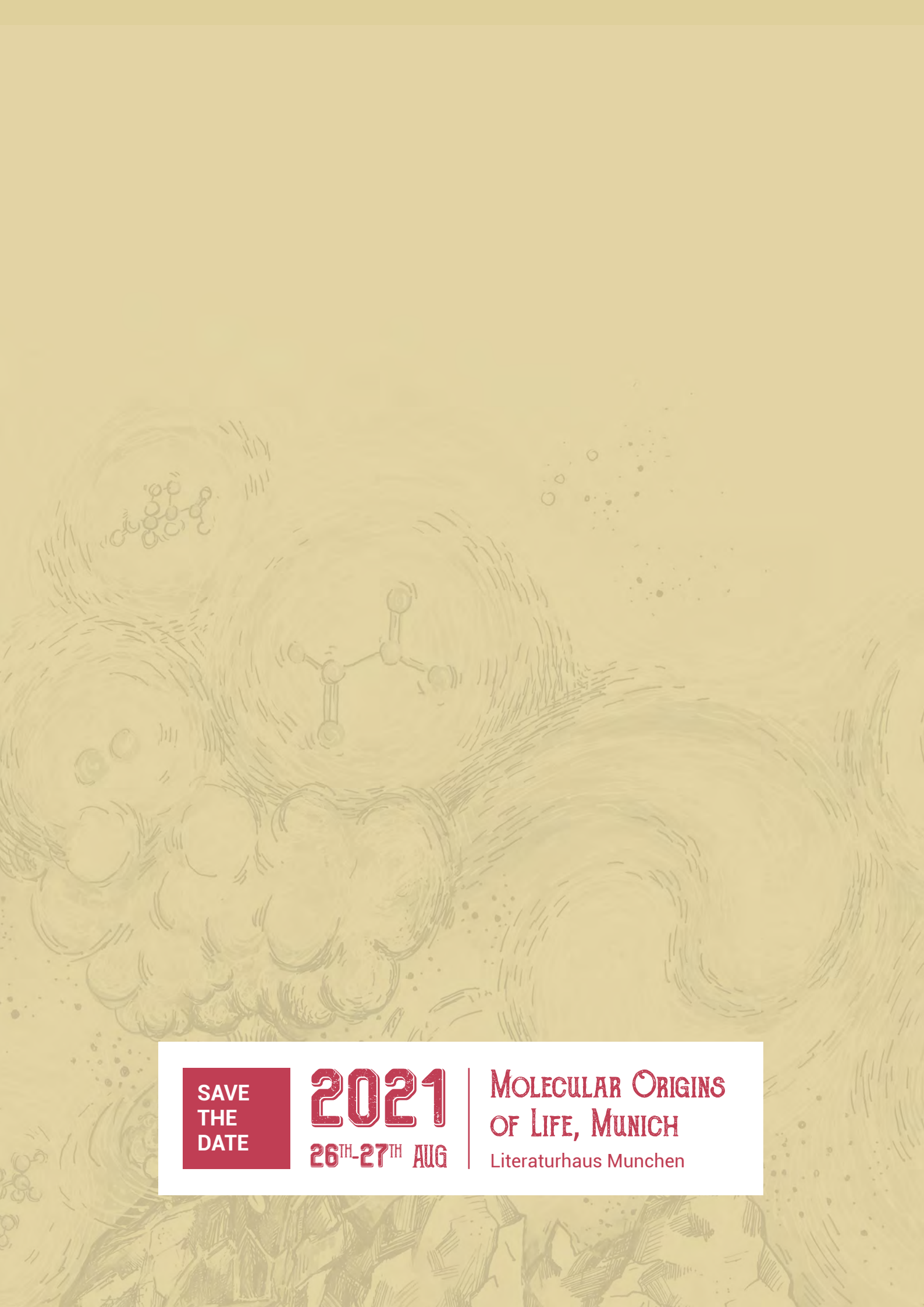
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