# The 29th annual meeting

**The 29th annual meeting of the society took place on April 17th, 2016**

# Program and Abstracts

## Program:

| Program of the 29th annual meeting | | |
|---|---|---|
| Time | Lecturer | Lecture Title |
| 8:45-9:05 | Refreshments & Gathering | |
| **Session 1 -Astrobiology (Doron Lancet, Chair; Amri Wandel, Organizer)** | | |
| 9:05-9:15 | Gonen Ashkenasy (BGU) | Opening Remarks |
| 9:15-9:45 | Ravit Helled (TAU) | Methane-Rich Planets and the Characterization of Exoplanets |
| 9:45-10:10 | Sohan Jheeta (NoR HGT, LUCA) | Formation of Glycolaldehyde (HOCH2CHO) from Pure Methanol in Astrophysical Ice Analogues |
| 10:10-10:35 | Joseph Gale (HUJI) | Is Liquid Water Essential for Life? A Reassessment |
| 10:35-11:00 | Coffee break | |
| **Session 2 - Evolution (Addy Pross, Chair)** | | |
| 11:00-11:40 | Robert Pascal (CNRS Montpellier) | Identifying the Kinetic, Thermodynamic and Chemical Conditions for Stability and Complexity in Living Systems |
| 11:40-12:05 | Omer Markovitch (Newcastle) | Predicting Proto-Species Emergence in Complex Networks |
| 12:05-12:30 | Amir Aharoni (BGU) | Engineering a Species Barrier in Yeast |
| 12:30-12:55 | Jayanta Nanda (BGU) | Spontaneous Evolution of β-Sheet Forming Self Replicating Peptides |
| 12:55-14:05 | Lunch | |
| **Session 3 - Origins of Order and Complexity (Gonen Ashkenasy, Chair; Tal Mor, Organizer)** | | |

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|---|---|---|
| 14:05-14:15 | Prof. Zvi HaCohen, Rector (BGU) | Greetings |
| 14:15-14:45 | Doron Lancet (WIS) | Composomics: a Common Biotic Thread |
| 14:45-15:10 | Avshalom Elitzur (IYAR) | Living State Physics: Does Life's Uniqueness Elude Scientific Definition? |
| 15:10-15:35 | Tal Mor (Technion) | Origins of Translation: Speculations about the First and the Second Code Word |
| 15:35-16:00 | Ilana Agmon (Technion) | Could Spontaneously Emerging Prebiotic Molecules Lead into Present Life? Could a Hurricane Assemble a Boeing 747? |
| 16:00-16:20 | Coffee break | |
| **Session 4 - Biochemistry and Prebiotic Chemistry (Omer Markovitch, Chair)** | | |
| 16:20-16:50 | Enrique Peacock-Lopez (Williams) | Chemical Self-Replication and Complex Dynamics in Open Systems |
| 16:50-17:15 | Yitzhak Mastai (BIU) | Chiral Selection on Inorganic and Organic Surfaces |
| 17:15-17:40 | Yifat Miller (BGU) | Self-Organization of Amylin Peptide with Absence and with Presence of Metal Ions: Mechanisms Related to Type 2 Diabetes |
| 17:40-18:05 | Miri Krupkin (WIS) | The Origin of the Ribosome: A Vestige of a Prebiotic Bonding Machine Functioning within the Contemporary Ribosome |

# Abstracts:

## Formation of Glycolaldehyde ($HOCH_2CHO$) from Pure Methanol in Astrophysical Ice Analogues

Sohan Jheeta (NoR HGT, LUCA)

The field of astrobiology is rapidly becoming a discipline in its own right as it seeks to answer the following questions: what are the conditions under which life can develop? How widespread are these conditions in the Universe? And, what are the mechanisms by which life evolves from basic 'building blocks' into self replicating systems?

It is believed that some of the necessary organic molecules may have been formed in the specialised areas of space (namely dark molecular clouds, eg Horsehead nebula) and delivered on to the Earth during the early period of its history, approximately 4.3-4.0 x $10^9$ years ago. These organic molecules may have played a pivotal role in the formation of life on Earth. In addition, it is believed that life on Earth was formed within a very short geological time frame of only 200-300 million years. So it is not unreasonable to suppose that these molecules were initially made in space as this could be, metaphorically speaking, a huge chemical laboratory.

The research being presented during this oral presentation focuses on the formation of glycolaldehyde ($HOCH_2CHO$) during the irradiation of pure methanol ice at 30 K with low energy electrons. This compound may have played an important role in the origins of life, since it may have been used in the synthesis of sugars (eg ribose) used in generating the necessary backbone of nucleic acids.

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# Is Liquid Water Essential for Life? A Reassessment

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## Lessons from Space and Earth

Water is a very common molecule in far and near space. Many of the Solar System Planet Satellites, such as Titan, Europa and Ganymede have as much or many times more water than Earth. From afar, Earth, 71% of whose surface is covered with water, appears to be a "water planet" teaming with life. However, <1% of its mass is water. Moreover, of the water in and on Earth >88% is lifeless. The mere presence of liquid water elsewhere in space cannot be an assurance of the presence of life. Life has many other requirements, foremost among them - a supply of free energy. Other solvents, such as hydrogen cyanide and formamide, that are liquid at common Earth temperatures, may also be candidates for bearing life.

Life on Earth evolved to utilize the special characteristics of liquid phase water, a physico-chemically exceptional molecule. These include internal structure, thermal stability, high dielectric constant, etc. However, some properties of water also constrained life. For example, water and the reduced iron salts dissolved in the primeval ocean, did not transmit radiation longer than 700nm. This allowed the evolving oxygenic photosynthesis to utilize less than half of the available solar energy; a restrictive adaptation that prevails even on dry-land based plants, today.

### A little Science Fiction speculation

Could there be life in solvent molecules that may be liquid, but not at Earth temperatures? For example, Titan, a satellite of Saturn, has clouds, rain, rivers and lakes, composed of methane, ethane and some tholins*. They are liquid at the prevailing surface temperature of about 94K. Any life, which emerged on the surface of Titan, would be much different to that on Earth. For example, its metabolic rate would be very slow, engendering extremely long lifetimes. For humans, a major limiting factor to space travel is our short longevity. However, for Titanians, trips lasting thousands of Earth years could be feasible, at least timewise!

*A large group of abiotic tar-like, complex organic solids, produced by irradiation of gases, such as $H_20$, $NH_3$, $CH_4$, etc., found on many Solar-system sites.

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## Identifying the Kinetic, Thermodynamic and Chemical Conditions for Stability and Complexity in Living Systems

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Thermodynamic stability usually drives the formation of complex molecular structures through favourable interactions that compensate for the entropy loss associated with the formation of adducts. Therefore it constitutes the usual driving force for the self-organization of chemical structures (e.g. crystals) as requested by the Second Law. As regards living organisms, association processes directly driven by the Second Law are common (e.g. the recognition of protein domains or that of nucleic acid strands as well as the assembly of the membrane). However, the drift towards the equilibrium state is not sufficient to explain the development of life through the evolutionary process. Maintaining a far-from-equilibrium state is essential for living organisms (Schrödinger, 1944), which requires open systems receiving low-entropy free energy from the environment. Populations of entities capable of multiplying themselves and able to grow accordingly can manifest another kind of stability associated with the power of exponential growth (Pross, 2012). These systems will be driven towards an increase in persistence (Pascal and Pross, 2015) as a result of their replication efficiency rather than directly through a spontaneous evolution towards the equilibrium state. This kind of stability, called dynamic kinetic stability (Pross, 2012) constitutes the driving force in a Systems Chemistry approach to the origin of life. It is associated with a requirement for kinetic irreversibility in the reproduction cycle in order that the mathematical logic of exponential growth becomes hegemonic over the diffusion of components and the evolution towards statistical distributions (Pascal and Pross, 2014; 2015). A combination of parameters was determined for systems having a wide range of generation times within orders of magnitude of seconds to years and at temperatures compatible with liquid water. This combination, consistently with the observation of life on Earth, involves reacting entities made of covalent bonds (i.e. compatible with organic chemistry) and fed in energy with a thermodynamic potential equivalent to that of visible light (Pascal, 2012a; 2013; Pascal et al., 2013).

### References

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## Predicting Proto-Species Emergence in Complex Networks

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Lognormal distributions are abundant in nature, e.g., distributions of earth's crust chemical and radioactive composition, latent periods of infectious diseases, abundance of bacteria on plants, olfactory receptors binding affinities, etc., have been shown to fit a lognormal distribution. Lognormal networks are graphs whose edge-weights follow a lognormal distribution. Here we utilise lognormal networks to analyse the emergence of "species" within an Artificial Life model of prebiotic evolution, based on the graded autocatalysis replication domain (GARD) simulator for prebiotic molecular assemblies. The temporal evolution of these assemblies is stochastically determined by a rates matrix - typically drawn from a lognormal distribution - that governs the likelihood that a given molecule joins or leaves an assembly. We re-interpreted here the rates matrix as a network and we analyzed its community structure. We asked whether communities are related (and how) to the evolved species under stochastic dynamic GARD and found that the derived communities correspond well to the species that emerge from the prebiotic evolution simulations. Importantly, we show that it is possible to predict proto-species emergence without performing any simulations. The analysis developed in this paper may have impact in other areas of Artificial Life, Complex Chemical Systems and Synthetic Biology.

## Spontaneous Evolution of β-Sheet Forming Self Replicating Peptides

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The study of non-enzymatic peptide replication reactions in the context of origin and the early evolution of life has drawn significant attention in recent years. In this respect, the self-assembly of β-sheet forming-peptides, and their replication propensity have been previously studied in our group.[1-2] It has been shown that short peptides having alternating hydrophobic (Phe) and hydrophilic (Glu) amino acids tend to form β-sheet-like structures[1-3], and can serve as efficient templates for self-replication.[1-2] In this case, the template molecule catalyzes the condensation reaction and native chemical ligation (NCL) between two short fragments, suggesting its unique ability to arrange themselves into well-ordered and defined structures.[1-2] However, in comparison to the Ala-Cys dyad leading to NCL, the ligation reaction at a Glu-Phe dyad proceeds through a completely different mechanism. In my presentation, I will show the replication reaction of β-sheet forming peptides that possess such Glu-Phe dyad at the ligation site. The mechanistic pathways for the evolution of four products will be demonstrated. This mechanism is explained by the formation of an intermediate glutaric anhydride, its epimerization, and consequently the attack of the nucleophile at the intermediates during the course of reaction. In template assisted reaction, addition of template primarily amplifies its own replication compared to other products due to better recognition. The self-assembly and self-replication of these prebiotically relevant peptides, suggest that such systems might have played a vital role in the Origins of Life.

### References

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## Composomics: a Common Biotic Thread

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Life's origin is about how sufficient chemical complexity emerged on early earth to afford replication. The graded autocatalysis replication domain (GARD) model (1), in the realm of the lipid world scenario (2), offers a novel route for these events, presumed to have taken place much before the advent of complex biopolymers, such as RNA. In this framework,

non-covalent assemblies of diverse amphiphiles, e.g. multi-component lipid micelles or vesicles, can acquire adequate endogenous complexity and harbor considerable inter-assembly variation. Our computer simulations show that GARD assemblies carry and transmit compositional information through homeostatic growth, mediated by a set of catalyzed chemical reactions akin to metabolism followed by random fission. Key in GARD dynamics are composomes, spontaneously-forming replication-prone states emerging through compositional dynamics. We have recently demonstrated that composome populations resemble the much-studied RNA quasispecies (4). We further showed that such GARD species display a significant measure of Darwinian selection and evolution, particularly when their catalytic networks are enriched in mutual-catalysis as opposed to self-catalysis (3). Finally, we found that composome populations portray ecological dynamics that fit the logistic equation, often used to analyze species transitions (3). Thus, the GARD formalism allows one to outline a well-defined chemically-rigorous path from random chemical environments ("primordial soup") to replicating and evolving protocellular structures, without a prerequisite appearance of RNA-like catalytic replicators. Future GARD studies will seek a quantitative delineation of the transition from compositional information to polymer-based sequence-based information, thus supporting the concept of metabolism as a precursor for RNA world. In this realm, we pursue the idea that a present-day living cell is a very elaborate compositional assembly, whereby well-orchestrated compositions of RNAs, proteins, lipids and metabolites define its identity. Thus, "composomics" is a term that unifies transcriptomics, proteomics, lipidomics and metabolomics, forming a bridge between a hypothesized prebiotic emergence path and the fully evolved present day cellular life.


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## Living State Physics: Does Life's Uniqueness Elude Scientific Definition?


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A famous debate ensued between Plato and Aristotle about form's alleged independence from matter [1]. Some years ago [2] I applied Plato's argument to the nature of life. It turns

out that a distinguished German-Israeli philosopher has made this argument long ago [3]. Replication and metabolism are processes where a physical body loses all its matter yet remains intact due to new incoming matter. To these formulations I add thermodynamics as the science that studies forms' assembly, stability and dynamics. Life's can thus be defined as a process where pure forms become causally effective qua forms, regardless of their material constituents. These forms interact with the corresponding aspects of their environment: When an environment is populated with numerous identical copies of the same form, natural selection adapts the form only to the environment's invariant, even abstract properties. Life then is a process where abstract, mathematical entities become increasingly liberated of the limits of their matter and energy, as well as of space and time boundaries.

Finally I revisit our earlier argument [4] about the time scale needed for the evolution of other biospheres in the universe. Matter, energy, space and time are the four basic physical parameters the likelihood of life's emergence and evolution. Abundance of the other three allows the time parameter to be orders of magnitude smaller.

**References:**


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## Origins of Translation: Speculations about the First and the Second Code Word


Tal Mor (Technion)



Based on Kauffman's notion of autocatalytic sets (ACS) we defined (ILASOL 2015, TPNC 2015) "code prompting autocatalytic sets" (COPACS) - sets of molecules and interations among them, that provide a model for artificial life, and could potentially provide a feasible explanation for the origins of translation. Here we discuss several possibilities for the first and the second code words, while considering RNA-peptide world versus RNA world.


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## Could Spontaneously Emerging Prebiotic Molecules Lead into Present Life? Could a Hurricane Assemble a Boeing 747?

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The likelihood of life arising spontaneously by natural processes is a major point of debate in human thinking. Fred Hoyle, an English physicist and cosmologist said that "the probability of life originating on Earth is no greater than the chance that a hurricane, sweeping through a scrapyard, would have the luck to assemble a Boeing 747" (Hoyle, F. Nature 1981).
Here, using basic principles mostly derived from the current biology, a simple Auto Catalytic Set of molecules and chemical processes is presented. The feasibility of the spontaneous emergence of such a set, which could have then continuously led from the prebiotic era into "life as we know it", i.e. into coded life based on amino acids and nucleic acids, is discussed.

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## Chemical Self-Replication and Complex Dynamics in Open Systems

Enrique Peacock-Lopez (Williams)

For many years it has been recognized that autocatalysis is necessary element for complex chemical oscillation. Chemical self-replication is one of the simplest cases of autocatalysis, and it has been experimentally studied for the lat twenty years, using organic compounds, nucleotides, ribozymes, and peptides. In most cases the experiments considered closed systems and were more interested in established possible chemical paths related to the origins of Life.

In parallel to the experimental analysis, we have proposed simple models of self-replication and analyzed its dynamics in open systems. In particular, we have analyzed Joyce's rybozyme experimental model and considered extension of self and cross-catalytic self-replication via a single template mechanism. In this case the dynamic behavior in open systems include chemical spatio-temporal patterns, but the limitation to a singlet catalytic species reduces he dynamic options and avoids complex catalytic self-replicating networks.

In contrast the formation of catalytic duplexes open up a myriad of possibilities in both closed and open systems. So far only peptide can be manipulated experimentally to select or design chemical self-replication via a catalytic active duplex. On the one hand, potentially, DNA may be able to self-replicate forming a triple helix, but experimental evidence of this mechanism is absent. On the other hand, artificial peptide networks have been synthesize and experimentally studied in batch reactors.

In our present work, we considered the dynamic analysis of self-replicating peptide systems that can use a singlet or a duplex as catalytic templates. In the case of open systems, we analyzed the coexistence of competitive self-replicating simple networks. Finally, we also consider the dynamics of recombinant peptides in artificial peptide networks.

## Chiral Selection on Inorganic and Organic Surfaces

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Among the most promising models for chiral selection of molecules, is based on adsorption on chiral crystalline surfaces that can select, concentrate and possibly even organize molecules into super-molecular structures. In this lecture we will review the various chiral inorganic and organic crystalline surfaces. The research in our group focuses on the use of chiral self assembled monolayers (SAM) for the preparation of nanosize chiral surfaces. In this lecture we present our novel approach for the preparation of inorganic cchiral surfaces with nano size of metal oxide surfaces of Titania ($TiO_2$) and Alumina ($Al_2O_3$) based on atomic layer deposition (ALD) onto chiral SAM[5]. Moreover we will present our results on the use of those chiral surfaces for few chiral applications. Finally we will review experimental and theoretical approaches to chiral selection on chiral inorganic crystalline surfaces that may open new frontier in understanding and exploiting chiral selection in nature.

## Self-Organization of Amylin Peptide with Absence and with Presence of Metal Ions: Mechanisms Related to Type 2 Diabetes

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The aggregation of amylin peptide is one of the symptoms of type 2 diabetes. The amylin peptides are self-assembled to oligomers that are toxic to β-cells and lead to their deaths. Metal ions are some of the factors that affect the self-assembly of amylin oligomers. The mechanisms through which amylin peptides are self-assembled with absence and with presence of metal ions will be presented. Our simulations show that there are various pathways in which amylin can self-assemble into oligomers, but metal ions decrease the number of pathways of self-assembly. Therefore, the self-assembly mechanisms of amylin with presence of metal ions demonstrate highly selective pathways.

# The Origin of the Ribosome: A Vestige of a Prebiotic Bonding Machine Functioning within the Contemporary Ribosome

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Ribosomes are the universal molecular machines that translate the genetic code into proteins. Peptide bond formation, the main catalytic activity of the ribosome, occurs in a universal semi-symmetrical region identified within all contemporary ribosomes, called by us the proto-ribosome. This region is composed solely of RNA with highly conserved sequence and structure.

Here, we examine the origin of the ribosome, suggesting it has evolved from an RNA entity that we named the “pre-proto-ribosome”. The suggested pre-proto-ribosome is a prebiotic pocket-like RNA apparatus capable of accommodating substrates in a way that enables chemical bonds formation. This pre-proto-ribosome, a molecular machine capable of performing essential tasks in the prebiotic RNA world, was later snatched for producing proteins by the amino acids invaders.

To experimentally explore this hypothesis, RNA constructs were designed based on the ribosomal sequence to mimic this universally conserved region. These RNA constructs have been in-vitro transcribed and were shown to dimerize as predicted from the structure of the ribosomal semi-symmetrical region. These RNA constructs have been subjected to binding assays, showing binding of small molecules that were potentially abundant in the RNA world. Designing an RNA machine capable of forming a peptide bond will demonstrate the missing link between the RNA world and our RNA-protein dominated world.

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and Humanities.

Key words: proto-ribosome, pre-proto-ribosome, RNA world.