AGENDA & BOOK OF ABSTRACTS

MONDAY 19 JULY, 2021, 10 AM – 12 PM

ZOOM ONLINE EVENT

AGENDA

10:00 – 10:10

Introduction (Julyan Cartwright – COST Action Chemobrionics chair)

10:10 – 10:30

Precipitation of Biomorph Fibers on Micropatterned SU-8 Posts (Pamela Knoll – invited speaker)

10:30 – 10:40

A Neural Network Framework for the Generative Modelling of Chemical Gardens (Thomas Chen)

10:40 – 10:50

Self-organization of biomimetic photo autotrophic protocell-like assemblies 'Jeewanu' in a laboratory simulated possible prebiotic atmosphere (Vinod Kumar Gupta)

10:50 – 11:00

Controlled formation of chemical gardens and the fabrication of chemobrionic materials (Erik Hughes)

11:00 – 11:10

Surface instabilities of tubular chitosan hydrogel (Pawan Kumar)

11:10 – 11:20

Reaction media for construction of a Belousov- Zhabotinsky chemical computer (František Muzika)

11:20 – 11:30

Interpreting communicating artificial cells by the MacKay theory of semantic information: a viable path? (Pasquale Stano)

11:30 – 11:40

Carbon-carrageenan ionic blends for application in soft robotics (Janno Torop)

11:40 – 11:50

Organic-to-inorganic transition of chemical gardens (Réka Zahorán)

11:50 – 12:00

CuS-Carrageenan nanocomposite Grown from the Interface of Gel/Liquid (Morad Zouheir)

The European COST Action Chemobrionics (CA17120) aims to link research groups to stimulate new, innovative and high-impact interdisciplinary scientific research on chemobrionics. It focuses on self-organizing precipitation processes, such as chemical gardens forming biomimetic micro- and nano-tubular forms. The main theme of the "Chemobrionics" workshop at the virtual conference on artificial life ALIFE 2021 will be to explore, quantify and understand non-equilibrium chemical systems, namely in the context of origin of life and artificial life.

The aim of the workshop is to bring together researchers interested in chemobrionics and wet artificial life, namely chemists, physicists, biologists, engineers. Further, it is expected that computer scientists performing mathematical simulations of life-like phenomena in chemical systems and experts from robotic field that build the platforms for laboratory experiments automatization will participate as well.

TOPICS

- Wet artificial life
- Origin of life
- Protocells
- Chemobrionics
- Messy chemistry
- Chemical garden
- Complex system
- Nonlinear physics
- Self-organization

ORGANISERS

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A NEURAL NETWORK FRAMEWORK FOR THE GENERATIVE MODELLING OF CHEMICAL GARDENS

THOMAS CHEN

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Currently, there is limited research in the area of chemobrionics, and specifically, the use of chemical gardens to inform future materials design. While synthetic biological approaches are useful for this purpose, recent advances in artificial neural networks and generative modelling have sparked discussions about using artificial intelligence techniques to model chemical gardens and predict their development. In this preliminary research, we discuss the use of generative adversarial networks (GANs) that are composed of the "indirect" training through the discriminator to model chemical gardens forming biomimetic micro- and nano-tubular forms. We seek to train on both imagery data and tabular data consisting of external features that represent the quantity and quality of items in the garden. A prospective future goal of this work is to also shed some light on the origin of life through observations of these chemical garden representations.

SELF ORGANIZATION OF BIOMIMETIC PHOTO AUTOTROPHIC PROTOCELL-LIKE ASSEMBLIES 'JEEWANU' IN A LABORATORY SIMULATED POSSIBLE PREBIOTIC ATMOSPHERE

VINOD KUMAR GUPTA

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Sunlight exposed sterilized aqueous mixture of some inorganic and organic substances showed photochemical formation of protocell-like microstructures, "Jeewanu" (Bahadur & Ranganayaki, 1970). The optical and scanning probe cytochemical investigations of Jeewanu showed that they are capable of multiplication by budding, grow from within and show various metabolic activities. They have been analysed to contain various compounds of biological interest viz. amino acids in free as well as in peptide combination, nucleic acid bases, sugars as ribose as well as deoxyribose and phospholipid like material in them. These microstructures can catalyse photolytic decomposition of water utilizing sunlight as a source of energy. Further it was found that hydrogen thus released in the mixture is utilized in the photochemical fixation of molecular nitrogen and carbon dioxide (Smith et.al.,1981). In the primitive atmosphere the function properties of molecules led to self-organisation of a specific group of molecules in specific stearic position and transformation of lifeless materials into emergence of earliest energy transducing system similar to Jeewanu.

References

Bahadur, K. and Ranganayaki, S. (1970) J. Brit. Interplanetary Soc. 23, 823.

Smith, A., Folsome, C. and Bahadur, K. (1981) Experientia, 37, 357-359.

CONTROLLED FORMATION OF CHEMICAL GARDENS AND THE FABRICATION OF CHEMOBRIONIC MATERIALS

[1,2] Erik A B Hughes, [1] Thomas E Robinson, [1] Richard J A Moakes, [1] Miruna Chipara and [1] Liam M Grover

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Chemobrionic systems typically result in the formation of self-assembling abiotic macro-, micro- and nano-material architectures. Chemical gardens are a classical example of a chemobrionic system characterised by the spontaneous formation of colourful hollow tubular precipitates following the introduction of metal salt seeds to reservoirs of anionic solution. From a technological perspective, chemobrionic processes may hold great promise for the creation of novel, compositionally diverse and ultimately, useful materials and devices. Challenges remain in controlling these reactions at a scalable manner and processing the resulting structures without breakage or loss of alignment. In this work, chemical gardens are grown from a hydrogel-solution interface housed within a customisable synthesis vessel. This platform was adapted with inlet and outlet channels such that reactant solution can be displaced. We demonstrate that systematic displacement of reactant solution with deionised water affords a means to cease chemical garden formation and purify the self-assembled tubular microstructures. Furthermore, displacement of purification media with a polymer phase provides a viable route for fabricating heterogeneous composite materials that incorporate chemobrionic components. Analysis of a chemobrionic composite by micro-computed tomography (µ-CT) and scanning electron microscopy (SEM) revealed aligned, high-aspect ratio channels running through an otherwise dense polymer matrix. This work sets a precedent for utilising chemobrionic principles to create technological relevant constructs, paving the way for the development of novel materials in a variety of application areas, such as regenerative medicine, catalysis and microfluidics.

PRECIPITATION OF BIOMORPH FIBERS ON MICROPATTERNED SU-8 POSTS

PAMELA KNOLL

Biomorphs are polycrystalline assemblies composed of metal carbonates and silica. They form smoothly-curved life-like shapes such as sheets, helices, funnels, and corals each composed of thousands of coaligned crystalline nanorods. Micrometer-sized posts composed of the photoresist epoxy SU-8 were photolithographed onto glass substrates and placed into the biomorph forming solution. These posts induced a new morphology reminiscent of fibrous, hair-like bundles that typically initiated along the perimeter of the cylindrical SU-8 material. Raman and energy dispersive X-ray spectroscopy show they are composed of barium carbonate with silica with similar ratios to classic biomorph structures. Scanning electron microscopy reveals that the hairs are composed of many thin strands coaligned along the direction of growth that expand through continuous fractal-like branching or abrupt splitting events. Biomorphs also formed on the glass substrate; however, following the collision with SU-8 obstacles the growth transformed into fibrous hairs and ultimately detached the posts from the glass.

SURFACE INSTABILITIES OF TUBULAR CHITOSAN HYDROGEL

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Spatial structures break their symmetry under the influence of shear stress arising from fluid flow. Here, we present surface instabilities appearing on chitosan tubes when an acidic solution of chitosan with various molecular weights is injected into a pool of sodium hydroxide solution. Wrinkling and folding patterns are monitored by varying the flow rates and container's orientation (vertical, inclined, and horizontal). The underlying wrinkling and folding instability are identified by its characteristic wavelength dependence on the depth of the tubular elastic material formed for the vertical configuration.[1,2] The mechanism for the transition of folding to wrinkling patterns relies on the compressive and axial stress on the CS tubules, which is validated by changing the angle of the inclined container. The flow-driven conditions allow precise control over the structure that can help the design of soft bio-inspired materials.

References

[1] P. Kumar, D. Horváth, and Á. Tóth, Soft Matter 16, 8325 (2020).

[2] P. Kumar, C. Hajdu, Á. Tóth, D. Horváth, ChemPhysChem 22, 488 (2021).

Acknowledgments

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REACTION MEDIA FOR CONSTRUCTION OF A BELOUSOV-ZHABOTINSKY CHEMICAL COMPUTER

FRANTIŠEK MUZIKA, JERZY GÓRECKI

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Our work is focused on assessing reaction media and resin types for construction of a Belousov- Zhabotinsky reaction chemical computer processing information assemblage with interacting oscillators, Gorecki et al. 2020 [1], made of catalyst loaded Dowex resins, controlled by application of an electric potential, creating information input interface between reactor and other devices. The electric field control technique was proposed by Kuze et al. 2019[2] using potentiostat on single Dowex resin with varying diameter, which became parameter limiting the type of oscillation either to travelling wave or global oscillation. The electric potential creates activator species for BZ reaction, $HBrO_2$, according to reaction: $BrO_3^- + 2e^- + 3H^+ \rightarrow HBrO_2 + H_2O$. The negative electric potential on working electrode attracts activator molecules $HBrO_2$, while positive electric potential is attracting inhibitor species Br^-. The reactor is batch type open to the atmosphere. The catalyst-free solution in the batch reactor was a mixture of concentrated sulphuric acid, $NaBrO_3$, and different ratios of malonic acid and 1,4 cyclohexanedione. We used three types of ferroin-loaded cation Dowex 50w beads (type x2, x4, and x8), which differ by their level of crosslinking, ion loading capacity, and size between 16 to 100 mesh. The influence of electric potential on a bead touching/not touching working electrode, and the influence of the number of adjacent beads and their spatial distribution on the oscillatory types and periods were investigated. The usual problem of BZ chemical computer, limiting their operation time to tenth of minutes, is formation of BZ reaction product, CO_2, in a form of bubbles, which create diffusion barriers and have ability to break the whole chemical computer assemblage by expanding force of gas. This problem is addressed by a choice of Dowex beads type, substrate type, and usage of highly concentrated acetone (Somboon et al. 2015[3]). The preliminary results show that we can produce oscillations with stable amplitude, the period between 20 seconds and 240 seconds, and in some cases, the oscillations lifetime exceeding 15 hours. The investigated medium seems to be a promising candidate for an experimental realization of chemical computer processing information assemblage with interacting oscillators and electric potential interface [1].

[1] Gorecki J., Bose A., Frontiers in Chemistry **8**, 2020, 580703; DOI=10.3389/fchem.2020.580703

[2] Kuze M., Horisaka M., Suematsu N. J., Amemiya T., Steinbock O. and Nakata S., J. Phys. Chem. A **123**, 4853−4857 (2019).

[3] Somboon T., Wilairat P., Müller S.C. and Kheowan On-U., Phys. Chem. Chem. Phys. **17**, 2015, 7114-7121

INTERPRETING COMMUNICATING ARTIFICIAL CELLS BY THE MACKAY THEORY OF SEMANTIC INFORMATION: A VIABLE PATH?

PASQUALE STANO

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Tremendous advancements in bottom-up artificial cell research have been reported, thanks to the attractiveness of ideas, tools, and approaches of bottom-up synthetic biology. The latter differs from conventional synthetic biology because it aims at constructing cell-like systems with minimal complexity from scratch, employing "modern" biomolecules such as DNA, RNA, ribosomes, enzymes, lipids, etc., or allegedly primitive molecules (fatty acids, ribozymes, short peptides, ...), or even completely artificial molecules (amphiphilic polymers, ad hoc designed transition metal-based catalysts, organo-catalysts, amphiphilic molecules, etc.). The entire field is experiencing a momentum and a wide variety of approaches are continuously reported. Among the various directions, one of the most attractive refers to the capacity of artificial cells of communicating with other artificial cells, or, intriguingly, with biological cells. The hybrid scenario (interfacing artificial and natural) resembles, in several aspects, well known situations in the realm of artificial agents, namely the dichotomy between natural intelligence and AI or between biological bodies and robots. Indeed, artificial cells have been recognized as the third pillar of the artificial technologies (hardware: robotics, software: AI, wetware: artificial cells). The importance of communicating artificial cell is not only theoretical: it can represent the operational layer to interface artificial cells and natural cells, thus contributing to smart nano-medicine vectors, and also for developing coordinated behaviour in populations of artificial cells (to generate a next-level of organization).When discussed from the molecular biology viewpoint, communicating artificial cells are just described qualitatively or semi-quantitatively according to the usual language of experimental biology. On the other hand, it is interesting to note that from a more rigorous engineering viewpoint, communicating artificial cells can be described according to the classic Shannon information and communication theory (encoding-sending-transmitting-receiving-decoding; transmission channel capacity; Shannon entropy; maximal likelihood estimation; etc.). In particular, a sub-field of communication engineering has recently born, called "molecular communication", dedicated to the development of mathematical models of such special type of messages that are the molecules. However, there is still another approach that can find inartificial cell research a powerful allied for future investigation. We refer to the MacKay semantic theory of information, which is ancient as the Shannon theory, but was overtook in early days of cybernetics by the Shannon theory because when the meaning of a message is put aside, a message can be exactly modelled by the objective tools of mathematics (while the meaning of a message was labelled as too subjective, i.e., context-dependent). Because MacKay semantic theory of information ultimately associates the meaning of messages to the dynamics they elicit within the receiver, and thus putting organization and the perturbations of the organization on the stage, an open question is whether or not modern synthetic biology approaches rooted in self-organization theories can be utilized to explore the MacKay theory of semantic information under a new perspective (potentially, an experimental one). Such a scenario would enrich the current modelling approaches to artificial cells, protocells, and in general to cell-like structure with claimed life-like properties, and possibly contribute to their theoretical understanding. In this contribution – which is far from being conclusive about the subject - I will present a brief summary and some preliminary ideas about the above-mentioned scenario.

CARBON-CARRAGEENAN IONIC BLENDS FOR APPLICATION IN SOFT ROBOTICS

JANNO TOROP

The presentation focuses on soft robotics and describes results on custom-shaped carrageenan actuators well-purposed for safe physical contact, usable in invasive procedures on living beings, handling of fragile objects and a potential to be designed with biomimicry in mind. Devices are discussed as candidates for actuated prosthetics or even creation of artificial muscles. Such applications on the border of robotics and biology would require biocompatibility and an interface for the neural control of movement, with such systems sometimes classified as the field of study of neurorobotics. Carrageenans are a family of algae-derived polysaccharides with a curious ability to gelate under the influence of cations. Their complete biocompatibility and biosustainable origins would make them good candidates for biofrendly actuator materials.

ORGANIC-TO-INORGANIC TRANSITION OF CHEMICAL GARDENS

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In the emerging field of chemobrionics, spatiotemporal chemical structures construct in far-from-equilibrium systems. In our experiments, when the pre-gel alginate solution is injected into the calcium salt solution, the sol-gel transition develops the budding and tubular hydrogel morphologies. Furthermore, the inorganic tribasic phosphate and organic alginate compounds are reacted with calcium ions competitively, and balloon-type structure forms at higher concentration of phosphate ions. The gelation process, electrochemical potential, and X-ray micro-CT characterizations yield the comparison of transition between the pure organic and inorganic-organic peculiarities. This precise control of the structures and material properties can be used in designing new functional materials.

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CUS-CARRAGEENAN NANOCOMPOSITE GROWN FROM THE INTERFACE OF GEL/LIQUID

MORAD ZOUHEIR, TAN-PHAT HUYNH

Chemical gardens (or chemobrionics) featuring typical micro- and nano-structures result from self-organizing precipitation processes. These processes allow not only the development of new methodologies to understand non-equilibrium chemical systems and the origin of life, but also the exploration of potential methods to drastically enhance future materials design. An interesting morphologies as well as physical and chemical properties have been found when chemobrionics evolves a gel/ liquid interface. A novel CuS-carrageenan nanocomposites grown from the interface between sulfide solutions (liquid phases) and Cu-ι-carrageenan gels was highlighted. Several parameters including pH, copper and carrageenan concentration of the hydrogel that influence the growth of the nanocomposite have been examined. The focus materials are the nanocomposites, obtained from the different pH conditions, which were purified and examined in detail using several characterization techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS). The structure, composition, properties as well as the growth mechanism of the nanocomposite have been studied. Additionally, the electrical conductivity of the nanocomposite was exploited to be used as a sensor of relative humidity and temperature.