BP 14: Poster Session I

Bacterial biophysics, computational biophysics, membranes and vesicles, synthetic life-like systems and origin of life, systems and networks biophysics

Time: Tuesday 10:00–12:30 Location: P3

BP 14.1 Tue 10:00 P3

The Role of Localized Metabolic Activity in Streptomyces Hyphae: An Agent-Based Approach — •Ricardo Santander[1], Denis Iliasov[2], Thorsten Mascher[2], and Vasily Zaburdaev[1] — [1]Max-Planck Zentrum für Physik und Medizin, Kussmaulallee 2, Erlangen — [2]Institut für Mikrobiologie, Zellescher Weg 20b, Dresden

The filamentous bacterium Streptomyces undergoes complex multicellular development characterized by hyphal growth and branching. Recent discoveries of LpdA-containing fluorescent foci within the hyphae suggest localized sites of elevated metabolic activity and ATP production. To investigate their influence on hyphal morphogenesis, we developed an agent-based model simulating key cellular components and their interactions.

Simulations reveal that localized ATP production and high consumption rates near the tips create spatial heterogeneity in metabolic activity. By adjusting model parameters, the model replicates typical growth patterns and hyperbranching phenotypes observed experimentally.

Our findings suggest that the spatial distribution of metabolic foci and localized ATP production influence Streptomyces morphology and multicellular organization.

BP 14.2 Tue 10:00 P3

Optically driven thermofluidic assembly of bacteria — •Desmond Joseph Quinn[1], Selina Hanisch[2], Rohan Karande[3], and Frank Cichos[1] — [1]Peter Debye Institute for Soft Matter Physics, Faculty of Physics and Earth Sciences, Leipzig University, Leipzig, Germany — [2]Helmholtz Center for Environmental Research (UFZ), Leipzig, Germany — [3]Biophysical Chemistry, Leipzig University, Leipzig, Germany

Bacteria in their planktonic state are known to assemble into biofilms in the vicinity of a solid surface. The complex cascade that results in the adhesion of the bacteria to the surface is usually triggered by the diffusion of bacteria to its vicinity. We propose a method that makes use of temperature induced flow fields and depletion interactions for the localized assembly and manipulation of bacteria. In addition to the physical interactions that contribute to the assembly process, the motility of the bacteria affects the assembly and can be altered by the induced temperature and altered distribution of molecules. We try to disentangle these effects by studying passive and active bacteria independently. We look at how motility parameters change in response to the fields induced by the laser, and how this in turn affects assembly. Such controlled assembly of bacteria could be useful for technological applications in bioreactors. In addition, our method provides a way of experimentally probing the effect of localized temperature, osmotic pressure, and flow fields on the motility of bacteria.

BP 14.3 Tue 10:00 P3

Growth and characterization of MoS2 nanowalls on Ti-based bone implants — •Rania Ennaciri, Axel Printschler, Christof Neumann, and Andrey Turchanin — Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany

Antibiotic resistance presents an important issue in the medicine field particularly in the context of bone replacement surgeries, where infections from antibiotic-resistant bacteria can lead to severe health complications and even fatalities. While titanium (Ti) is the conventional choice for bone implants, there is a clear need for further improvements of this material to enhance its antimicrobial resistance. In this regard, hybrids based two-dimensional (2D) materials, such as molybdenum disulfide (MoS2), present a great promise due to their intrinsic antimicrobial activity and biocompatibility. These properties are generally manifested through biochemical reactions, by the generation of reactive oxygen species (ROS) that can lead to the damage of bacteria DNA, proteins and lipids. Also, mechanical actions, where the sharp edges of the nanowalls can cut the bacteria wall can lead to its death. To investigate these mechanisms, we use metal-organic chemical vapor deposition (MOCVD) technique to grow different morphologies and sizes of MoS2 nanowalls on Ti implants. We use scanning electron microscope (SEM), Raman spectroscopy and X-ray electron microscopy (XPS) to characterize the structural and chemical properties and to correlate them prospectively with the antimicrobial properties as well as with the growth bone cells.

BP 14.4 Tue 10:00 P3

Infrared Hyperspectral Mapping of Biofilms Growing in Confinement — •Felix Hermann Patzschke[1], Valentina Schmitz[2], Rohan Karande[2,3], and Frank Cichos[1] — [1]Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig — [2]Leipzig University, Institute for Biochemistry, Johannisallee 21-23, 04103 Leipzig — [3]Helmholtz Centre for Environmental Research, Permoserstraße 15, 04318 Leipzig

Biofilms are microbial communities characterized by complex spatial organization and dynamic chemical composition. The formation and growth of biofilms in confined environments are of significant interest in fields such as medicine and bio-engineering. We seek to establish a clearer understanding of the interplay between physical confinement and microbial behavior by investigating whether specific quantifiable aspects of a cavity's geometry can influence the likelihood of biofilm initiation and the rate of its growth.

We utilize Photothermal Infrared (PTIR) hyperspectral microscopy to acquire infrared spectral data at sub-cellular spatial resolutions. Through spectral decomposition, we aim to map the chemical composition of biofilms and distribution of nutrients in space and time. Our results provide a detailed view of biofilm structure, metabolic activity, and growth dynamics in confined settings. This work underscores the potential of PTIR microscopy as an impactful tool for advancing the understanding of biological systems in scientifically and technologically significant domains.

BP 14.5 Tue 10:00 P3

Self-Organized Colonization Resistance without Physical Barriers — •Christian Westendorf[1], Valentin Slepukhin[1], Birgit Koch[1], Victor Peris[1], and Oskar Hallatschek[1,2] — [1]Peter Debye Institute for Soft Matter Physics, Leipzig University. — [2]Department of physics, University of California, Berkeley.

Small micrometer-scale cavities, such as gut crypts, soil pores, and plant apoplasts, represent key bacterial habitats, in which different strains compete for resources and space. Recent studies have shown that the physical structures of these microhabitats can influence the stability and resilience of bacterial colonizers by protecting local populations from invasion. Building on this, we experimentally and computationally investigate the dynamics of mixed bacterial populations within interconnected microfluidic cavities, examining the influence of geometric features and surface interactions on microbial organization and diversity. Our findings reveal that surface roughness and friction can drive self-organization into effectively isolated subpopulations, safeguarding slower-growing strains from competitive exclusion. By comparing velocity fields of growing populations with stochastic and analytical simulations, we demonstrate how local geometry and emergent microhabitats balance selective pressures, maintaining microbial diversity under competitive and evolutionary stress. Our work suggests that colonization-resistant microhabitats can form dynamically, even in the absence of physical barriers.

BP 14.6 Tue 10:00 P3

Comparing graphene and 2D MoS_2 nanopores for protein translocation and detection — •Peijia Wei, Mayukh Kansari, and Maria Fyta — Computational Biotechnology, RWTH Aachen University, Worringerweg 3, 52074 Aachen, Germany

Nanopores, nanometer-scale openings in materials, have shown their strong potential in realizing ultra-fast, cost-effective, and real-time next-generation sequencing technology. These nanopores can electrophoretically drive charged biomolecules and detect these. Using computer simulations, we compare two-dimensional nanopores, namely graphene and MoS_2, to evaluate their effectiveness in protein detection. We modulate protein translocation and dynamics by adjusting the type and concentration of the surrounding solvent, using a typical

monovalent salt solution and a molecular solution. Utilizing atomistic simulations, we assess the efficiency of both nanopores in threading proteins, based on measurable ionic current signals. Our results show that graphene nanopores strongly interact with proteins, hindering translocation under physiological conditions. This issue is addressed by introducing a denaturant, which creates a hydrophilic-cationic layer on the pore surface, facilitating the linearized threading of proteins. In contrast, MoS_2 nanopores facilitate protein passage even in physiological solutions, offering an alternative approach to controlling translocation speed. We analyze the two nanopore materials based on molecular interactions among the material, protein, and solvent, emphasizing their impact on protein dynamics and ionic signal enhancement for efficient 2D nanopore protein detection.

BP 14.7 Tue 10:00 P3

Exploring coarse graining RNA force fields via Machine Learning — •Anton Dorn[1] and Alexander Schug[1,2] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]KIT Scientific Computing Center, Karlsruhe, Germany

In Protein structure prediction there have been massive improvements recently with the help of machine learning. In RNA structure prediction however the situation is less ideal due too much sparser experimental data. Here we attempt to solve a modified version of the problem by determining a coarse-grained RNA force field for Molecular Dynamics simulations. The data sparsity can here be alleviated by atomistic RNA simulations using proven and established force fields. In a first step we show the viability of this approach with a limited scenario of only small RNA molecules. For this we adapt the invariant Graph Neural Network architecture, cgSchnett.

BP 14.8 Tue 10:00 P3

Parameterization of a dissipative particle dynamics thermostat (DPD) thermostat for coarse-grained molecular dynamics — •Karan Venkatesh, Viktor Klippenstein, and Nico F. A. van der Vegt — Technische Universität Darmstadt

Coarse-grained (CG) simulations represent a viable approach for modelling dynamics on long length and time scales inaccessible with atomistic simulations. In this work, we present a single-site coarse-graining method designed to match the dynamical and structural properties of a molecular liquid (cyclohexane).

We employ a DPD thermostat, in which the pairwise forces are decomposed into parallel and perpendicular components. An iterative optimization scheme is implemented to parameterize the parallel and perpendicular forces, aiming to match the diffusion coefficient and shear viscosity of the system, respectively. In our study, we find that matching the diffusion coefficient also leads to a match in the shear viscosity. However, this correspondence may not always hold, especially when dealing with structurally anisotropic molecules and soft potentials, as commonly encountered in soft matter systems. This approach can be further extended to simulate mixtures of CG molecular liquids, and study penetrant dynamics in CG polymer melts.

References: 1. V. Klippenstein; N F A van der Vegt; J. Chem. Theory Comput. 2023, 19(4), 1099-1110. 2. M. Tripathy; V Klippenstein; N F A van der Vegt; J. Chem. Phys. 2023, 159(9) 3. C. Junghans; M. Praprotnik; K. Kremer; Soft Matter 2008, 4(1), 156-161

BP 14.9 Tue 10:00 P3

Leveraging Experimental Vasculature Data for High Resolution Brain Tumor Simulations — •Eric Behle[1], Julian Herold[2], and Alexander Schug[1] — [1]NIC Research Group Computational Structural Biology, Jülich Supercomputing Centre, Jülich Research Center, Jülich, Germany — [2]Steinbuch Centre for Computing, KIT, Karlsruhe

Cancer remains a leading cause of mortality. Multidisciplinary studies probe its pathology to increase treatment options. Computational modeling of tumors on HPC resources offers insight into its progress and an avenue for advancing our understanding. However, initialization and parameterization of the underlying models require high-resolution data from real tissue structures. Here, we leveraged HPC resources and a massive dataset of a mouse brain's entire vascular network. We processed these image stacks into detailed 3D representations, identified brain regions of interest, and conducted a series of large-scale simulations to investigate how tumor growth is influenced by local vascular network characteristics. By simulating tumor growth with sub-cellular resolution, we can probe to which extent vessel density and network length influence growth. We determined that vessel density is the primary determinant of growth rate. Finally, our results allowed us to extrapolate tumor cell growth predictions for the entire mouse brain, highlighting the critical role of vascular topology in tumor progression. Such increasingly realistic simulations of cancer cells may enable researchers to bridge the gap between basic biology and clinical practice, supporting development of cancer therapies.

BP 14.10 Tue 10:00 P3

Boundary integral method for elastic solids in Stokes flow and applications in real-time deformability cytometry — •Thomas Mayr and Stephan Gekle — Universität Bayreuth, Deutschland

A Newtonian fluid at small Reynolds numbers can be described using the Stokes equation. A common choice to solve the Stokes equation numerically is the boundary integral method. Previously, this method was mainly used to describe rigid particles or capsules with an elastic membrane such as red blood cells. Here a technique is presented how to extend the boundary integral method to elastic solids discretized by the finite element method. This can be used as simple model to describe the stiffness of cells with a nucleus and a cytoskeleton, e.g. in some deformation experiments. In our case we will compare the simulations with an experimental technique called real-time deformability cytometry (RT-DC).

BP 14.11 Tue 10:00 P3

Mathematical Modeling of Intercellular Calcium Waves in Fibroblast Networks — •Kara Nachtnebel — Isarstr, 6, 93057 Regensburg

Inflammatory responses are essential for defending against pathogens but can result in tissue damage when not properly regulated. Resident tissue macrophages (RTMs) play a crucial role in maintaining immune homeostasis by modulating inflammatory cascades. Disruptions in these regulatory mechanisms can lead to heightened immune responses and may contribute to the development of autoimmune diseases. This study explores the role of fibroblast networks and their calcium signaling dynamics in maintaining tissue homeostasis. We aim to understand the mechanisms underlying these dynamics and predict calcium signal propagation in both healthy and pathological tissues. A mathematical model is developed to describe intracellular calcium ion diffusion and Inositol-1,4,5-triphosphate (IP3) signaling in fibroblast cells interconnected by gap junctions (GJs). This model incorporates intracellular calcium stores and IP3-sensitive receptor (IPR) dynamics, which significantly influence calcium release into the cytoplasm. IP3 generation is modeled as a function of phospholipase-C (PLC) activation, triggered either by external stimuli or by calcium, leading to calcium-induced calcium release (CICR). Our approach provides insights into how calcium signaling networks contribute to tissue homeostasis and how their dysfunction occurs in pathological conditions.

BP 14.12 Tue 10:00 P3

coarse-grained simulations of Lge1(1-80) peptide. — •Agaya Johnson[1], Anton Polyansky[2], Pedro Sanchez[1], Bojan Zagrovic[2], and Sofia Kantorovich[1] — [1]Computational and soft matter physics, University of Vienna, Kolingasse 14-16, 1090, Vienna, Austria. — [2]Department. of structural and computational biology, Campus- Vienna-biocenter 5, 1030 Vienna, Austria.

Biomolecular condensates in cells such as p-bodies, nucleoli and stress granules play an important role in regulating biological processes like transcription and ribosome biogenesis. Studying of such biomolecular condensates will give insight into the molecular basis of disease, like neurodegenerative diseases, cancer and diabetes. The main purpose of this study is to understand the main phenomenon, which leads to the formation of these biomolecular condensates such that we get a conclusion, whether is it phase separation, self-assemble or an aggregation. We use Lge1(1-80) peptide as a model for study because Lge1(1-80) is mostly disordered prone to form many cation - pi and pi - pi interaction (R, G and Y rich sequence) and because of its alternating net charge which are the prerequisites for the phase separation. Due to the limitations of high-resolution experimental techniques, we are using molecular dynamics simulation with coarse-grained approaches with the help of software package ESPResSo. Our goal is to develop a coarse-grained model for proteins that exhibit structural transitions and to understand fundamental mechanisms under those transitions.

BP 14.13 Tue 10:00 P3

Optimizing a Biomimetic Cross-Flow Microplastics Filter Inspired by Manta Rays — •Ioannis Gkekas[1] and Tim Robertino Baumann[2] — [1]Universität Bielefeld — [2]Universität Bielefeld

Microplastic pollution poses a significant threat to aquatic ecosystems, necessitating innovative filtration solutions. This study continues previous research on a biomimetic cross-flow filter inspired by manta ray feeding mechanisms. The objective is to optimize the filter's geometry and material properties to enhance efficiency and durability. Using COMSOL simulations, various geometrical configurations are being tested to identify an optimal design for maximizing filtration efficiency and clean water output. To address material durability, we reenforced PDMS (polydimethylsiloxane) with glass fibers to mitigate bursting under operational stress. Initial results indicate that the composite material significantly enhances durability compared to the original PDMS design. Once the simulations are complete, the optimal design will be fabricated for in-lab performance evaluation. This research advances the development of sustainable, high-efficiency microplastic filtration systems inspired by natural processes.

BP 14.14 Tue 10:00 P3

Autonomous, intrinsic circadian oscillator at cell membranes — •Mauro Ariel Forlino[1], Oreste Piro[2], and Martín García[1] — [1]Universität Kassel, Kassel, Germany — [2]Universtat de les Illes Balears, Palma, España

Circadian rhythms originated in endogenous cellular clockworks are the evolutionary solution that allows organisms to anticipate and synchronize their internal processes with the predictable changes in their environment on a daily basis. According to the conventional paradigm, eukaryotic cells generate circadian rhythms as outputs from gene-based biochemical oscillators comprised of transcription/translation feedback loops, necessarily involving processes occurring within the nucleus. However, mounting evidence has recently emerged indicating that circadian rhythms also exist in cells devoid of such nuclear clocks, notably seen in the circadian variation of red blood cell metabolism. Here, we demonstrate the existence of a completely different mechanism for generating endogenous circadian oscillations that solely involves processes within the cell membrane and its immediate vicinity, entirely independent of the nuclear clock. Rather than relying on the transcription/translation/repression loop as in nuclear oscillators, this membrane-located clock operates through an analogous regulatory circuit that involves the homeostatic regulation of ion channels and their gating kinetics.

BP 14.15 Tue 10:00 P3

Influence of the sapogenin gypsogenin on vesicles from 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) — •Melanie Gettinger and Thomas Hellweg — Physical & Biophysical Chemistry, University Bielefeld, Bielefeld, Germany

Small unilamellar vesicles (SUVs) composed of phospholipids, such as 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC), are commonly used as model membrane systems. DMPC bilayers undergo phase transitions from a gel to a fluid phase at around 24°C. While the effects of saponins on DMPC membranes are well-documented, the impact of their aglycones, sapogenins, remains less explored. Gypsogenin, a pentacyclic triterpenoid found in soapwort (Saponaria officinalis) and gypsum herb (Gypsophila oldhamiana), is of interest due to its anti-cancer potential. Gypsogenin shares structural features with cholesterol but has contrasting effects on membrane properties. While cholesterol increases membrane thickness and reduces fluidity, gypsogenin incorporation decreases the vesicle core radius and membrane thickness, as shown by small-angle X-ray scattering (SAXS) and cryo-TEM. UV-vis spectroscopy was used to monitor turbidity in solutions containing 0 to 25 mol% gypsogenin over a wide temperature range, showing a reversible increase upon cooling, indicating thermally reversible phase transitions. SAXS measurements revealed significant structural changes at 25 mol%. The core radius and membrane thickness decreased compared to pure DMPC vesicles. These findings suggest that gypsogenin alters DMPC membranes significantly at higher concentrations.

BP 14.16 Tue 10:00 P3

Properties of Long-Chain Lipid Enriched Regions in Biological Membranes: Insights from MD Simulations — •Annemarie Quas, Clara Rickhoff, and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster

Experimental studies of yeast plasma membranes reveal gel domains enriched in long-chain lipids and depleted in ergosterol [1]. To explore these findings, we perform coarse-grained molecular dynamics simulations of membranes with varying concentration of long-chain lipids. To enhance our understanding, we simulate both asymmetric membranes with long-chain lipids in the outer leaflet, as observed experimentally, and symmetric membranes containing long-chain lipids in both leaflets. Our analysis focuses on characterizing key membrane properties and examining the influence of long-chain lipids. The role of ergosterol is also investigated. Additionally, we assess non-affine lipid movements to provide insights into the dynamics within these gel domains. This study aims to bridge experimental observations with molecular-level mechanisms, advancing our understanding of gel-phase organization and its implications for membrane functionality.

[1] Aresta-Branco *et al.*, *J. Biol. Chem.* **2011**, 7, 5043-5054

BP 14.17 Tue 10:00 P3

G-FETs for label-free biosensing of protein interactions — •Florian Steinbach, Mykola Fomin, Margarete Schwirblat, and Carola Meyer — Institute of Physics, University of Osnabrück, Germany

Graphene field-effect transistors (G-FETs) offer a promising approach for label-free biosensing due to their sensitivity and compatibility with liquid environments. In this work, we investigate liquid-gated G-FETs functionalized with lipid monolayers for detecting protein interactions at membrane interfaces.

The fabrication process was refined to improve device stability and reduce measurement variability. To enable reusability, we employed tris-NTA-functionalized lipids, allowing reversible binding and elution of hexahistidine (H6)-tagged proteins while preserving device functionality for subsequent detection cycles. Adjustments to the functionalization protocol included histidine-based elution, which better preserved the passivation layer compared to standard imidazole methods. Electrical measurements were used to monitor functionalization steps and protein interactions. Using monomeric enhanced green fluorescent protein (H6-mEGFP) as a model system, we present characteristic shifts and changes in transconductance during each step of the protocol.

These developments contribute to the optimization of G-FETs for biosensing applications, with particular attention to the stability of functionalized interfaces under physiological conditions. The findings will be discussed in the context of improving sensor design and extending the approach to more complex biomolecular systems.

BP 14.18 Tue 10:00 P3

Theory of spatial aggregation and shell formation — •Pranay Jaiswal, Ivar Haugerud, and Christoph Weber — Institute of Physics, University of Augsburg, Augsburg, Germany

Many biological systems use coexisting phases composed of proteins and RNA to regulate chemical processes and molecular transport. In particular, the interface can act as a nucleation site for aggregation of proteins, leading to the formation of a solid-like shell. This shell provides a physical barrier for molecular transport of further biomolecules, giving rise to molecule-specific interface permeabilities. Here we propose a theoretical model for spatio-temporal protein aggregation in phase-separated systems. To this end, we use a phase-field of proteins and RNA combined with a phase-field characterising the solid-like, aggregated state. Our key finding is that aggregation is thermodynamically favored at the interface, making aggregation shells a likely phenomenon in phase-separated systems of aggregation-prone proteins. We show how such aggregation shells control molecular transport and shell permeabilities. Our theory can be applied to experimental systems undergoing irreversible aggregation to unravel the molecular mechanism underlying ageing in protein mixtures.

BP 14.19 Tue 10:00 P3

Cell-free protein synthesis measured in flowing nanolitre-droplets — Benno Schedler[1], Alexandros Katranidis[2], and •Jörg Fitter[1,2] — [1]AG Biophysik, I. Physikalsiches Institut (IA), RWTH Aachen University, D-52074 Aachen, Germany — [2]Forschungszentrum Jülich, ER-C-3, D-52425 Jülich, Germany

Cell-size confinement of biological reactions by utilizing microfluidic water-in-oil droplets has been widely used to revolutionize the field of biomolecular research. This approach capitalizes on the precise control and manipulation of nanoliter-sized droplets within microfluidic channels. The confinement facilitates reduced reagent consumption and improved scalability. Analysing cell-free protein synthesis (CFPS) is an ideal application of this approach and represents a complex multistep process which can be monitored in individual droplets if fluorescent proteins are synthesized [1]. Understanding the physicochemical principles underlying CFPS reactions, including the role of macromolecular crowding, is crucial for optimizing protein synthesis yields and func-

tionality [2]. Here we present the results of our ongoing research using the example of the synthesis of green fluorescent protein (GFP), which we have analysed employing confocal fluorescence microscopy. Focus is set on the high throughput capability of the approach and thus the possibility of analysing several hundred parallel reactions. The latter provide important information about the average synthesis productivity and the distribution widths for reactions under different environmental conditions. [1] Hansen et al., 2016, Nature Nanotechnology, 11, 191; [2] Kempf et al., 2017, Scientific Reports, 7, 46753

BP 14.20 Tue 10:00 P3

Enhancing polymerization of prebiotic building blocks by wet-dry cycling — •Almuth Schmid and Dieter Braun — AG Braun, LMU Systems Biophysics, Munich, Germany

Prebiotic chemistry is limited by several factors as concentration or availability of starting materials on the early Earth. On top of that, many artificial and natural activation agents are too complex to have been a part of prebiotic reaction networks. To overcome this problem, amino acids might help reaching ideal environmental conditions, enhancing prebiotic reactions like polymerization of nucleotides. Preliminary experiments demonstrated, that in a wet-dry cycling system rel. yields of GC polymers are boosted up to 70% in the presence of amino acids.

By using wet-dry cycles and including other prebiotic plausible activating agents like volcanic rocks, a better control of the polymerization can be accomplished. Tracking the polymerization on tholeiite basaltic rock with SEM reveals first hints on where and how the polymers interact with the mineral.

BP 14.21 Tue 10:00 P3

Phase-separation enhances sequence selection via templated ligation — •Manav Koul, Ivar Haugerud, and Christoph Weber — Universität Augsburg, Universitätsstraße 2, 86159 Augsburg

The emergence of highly selective catalytic sequences was a crucial step towards the origin of life. templated ligation of RNA has been proposed as a pre-biotic mechanism to achieve self-replicating sequences without complex machinery. A question remains as to how sufficiently long and abundant templates can emerge from short nucleotides in a non-conducive prebiotic pool. As phase separation has been shown to provide versatile hubs of correlated sequences, we investigate its role in facilitating and directing templated ligation. To this end, we develop a non-equilibrium thermodynamic model to describe the oligomerization of sequences and their ligation at non-dilute conditions in phase-separated systems. We find that phase-separation enhances the selection pressure of this mechanism, resulting in a sequence distribution dominated by highly structured sequence of low entropy. Our results highlight that out-of-equilibrium condensed phases could provide versatile hubs for Darwinian-like evolution toward functional sequences, both relevant for the molecular origin of life and de-novo life.

BP 14.22 Tue 10:00 P3

Phase Transitions in Non-Hydrated DPPC Lipid Bilayers Deposited on Silicon: Effects of Dry Nitrogen Atmosphere and Thermal Cycling — •Nicolás Moraga[1], Daniel Saavedra[1], Nancy Gomez-Vierling[1], Marcelo A. Cisternas[2], María José Retamal[3], and Ulrich G. Volkmann[1] — [1]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]Escuela de Ingeniería Industrial, Universidad de Valparaíso, Chile — [3]Facultad de Ingeniería, Universidad Finis Terrae, Santiago, Chile

This study investigates the phase behavior of DPPC lipid bilayers in a non-hydrated state, deposited on silicon substrates, under conditions that are both experimentally innovative and highly relevant for applied science and fundamental research. By assembling these bilayers in vacuum and exposing them to dry nitrogen atmospheres, we present a novel platform that extends beyond classical hydrated systems, with significant implications for biosensing technologies. Through controlled thermal cycling using high-resolution ellipsometry, a technique offering exceptional sensitivity to subtle changes, we analyze phase transitions, uncovering the impact of hydration-free environments on lipid bilayer organization. These findings provide new insights into the thermal resilience of DPPC bilayers, highlighting potential phase stability domains. Additionally, this approach simulates extraterrestrial-like conditions where water is absent, underscoring the adaptability of lipid-based structures and advancing our understanding of molecular organization under vacuum and inert atmospheres. Acknowledgements: ANID Fellowships (NM, DS, NGV); Puente UC 2024-25.

BP 14.23 Tue 10:00 P3

Cooperative Effects in Compartmentalized Irreversible Self-Assembly — •Severin Angerpointner, Richard Swiderski, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Germany

From biomolecular compartments, protein patterns to porous rocks: Many biological and chemical systems like living cells or prebiotic chambers exhibit some form of spatial organization which separates biochemical processes. This is known to play a key role in the assembly of virus capsids or the enrichment of prebiotic chemicals. We systematically explore the effects of such spatial separation on the self-assembly of irreversibly binding identical particles. We show that already in a simplified model of two coupled biochemical compartments cooperative effects emerge through limiting compartment exchange. Further, these findings generalize to spatially extended systems like intracellular chemical gradients or membrane-assisted assembly.

BP 14.24 Tue 10:00 P3

Mathematical modelling of immune response on the example of psoriasis — •Nadezhda Esenkova[1,2], Lukas Pöschl[1,2], Gerard C. L. Wong[3], and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [3]University of California, Los Angeles, USA

In recent years it was shown that antimicrobial peptides (AMPs) can contribute to the immune response by triggering Toll-Like Receptors (TLRs) on immune cells. Apart from natural AMPs it was suggested that proteolytic enzymes, secreted by neutrophils can digest other signaling molecules to AMP-like fragments, which can stimulate immune response and lead to disease progression. The goal of this work is to create a mathematical model of immune response by introducing this novel link of AMP-like fragments. To this aim we constructed a comprehensive signaling network of the immune response based on one of the best studied autoinflammatory diseases – psoriasis. Taking into account the key biological pathways we reduced it to the core network model, which we investigate using theoretical dynamical systems analysis and modern machine learning methods. We aim to understand how the hypothesized mechanism of autoinflammation due to AMP-like fragments augments the disease outcomes from full resolution, to chronification and rapid exacerbation.

BP 14.25 Tue 10:00 P3

Formation of thermally driven pH gradients from salts — •Riccardo Schiroli, Thomas Matreux, and Christof B. Mast — Systems Biophysics, LMU München, Munich, Germany

The impact of pH on biomolecule stability and chemical reactions suggests its crucial role in prebiotic chemistry. Thermophoresis, the movement of molecules along a thermal gradient, has been shown to accumulate and select a wide range of biomolecules, including RNAs and amino acids as well as different salt species leading in specific conditions to the emergence of pH gradients.

In this study, we investigated the formation of heat flow driven pH gradients in simulated rock fissures under various experimental conditions, including different salt solutions, initial pH values, and temperature gradients. Ion chromatography, combined with complexation techniques and fluorescent analysis, was used to analyze the distribution of ions and pH profiles within the fissures.

Our findings show that heat flows can efficiently induce pH gradients in solutions containing various salt species. We observed significant accumulation of common ions, leading to pH gradients in both alkaline and acidic solutions. Furthermore, we found that certain metal ions, such as lanthanides and iron, can significantly enhance the formation of pH gradients, even at micromolar concentrations. This study provides evidence for the role of heat flows in creating localized pH gradients under prebiotically plausible conditions. Our results highlight the ease with which pH gradients can form under a wide range of prebiotic plausible conditions, driven by simple heat flows.