12th Christmas Biophysics Workshop

Book of Abstracts

Golte, Slovenia, December 11-12 2017

organized by Jožef Stefan Institute

edited by Jan Rozman and Primož Ziherl

Foreword

Organized every year since 2006, the Christmas Biophysics Workshops have evolved into small but focused meetings providing a regional forum for biophysicists from Austria, Croatia, Italy, and Slovenia. These meetings are especially important because of the numerous collaborations among researchers from the four countries, many of which have been initiated or are maintained at these Workshops. We have all appreciated the rather informal but productive style of the past ten events held in Zagreb, Bled, Donja Stubica, Leibnitz, Ptuj, Varaždin, Riegersburg, Buzet, San Daniele, Sankt Nikolai, and we hope that you will find the Golte Workshop just as enjoyable.

Jan Rozman and Primož Ziherl

Program

Monday December 11 2017

9.00-10.00 Arrival and registration

10.00-11.20 Biopolymers I (chair: Rudolf Podgornik)

10.00 Vojtěch Mlýnský: *Modeling RNA interactions with SHAPE reagents*
10.20 Lucia Coronel: *Simulations of supercoiled DNA rings*
10.40 Adela Štimac: *FCS testing of DNA interaction with cyclodextrine based supramolecular systems functionalized with adamantyl guanidine*
11.00 Sabine Reißer: *Conformational ensemble of an RNA hairpin: A combined maximum entropy and maximum parsimony approach*

11.20-11.50 Coffee break

11.50-13.10 Lipids, membranes, and vesicles (chair: Cristian Micheletti)

11.50 Moritz Frewein: *Intrinsic lipid curvatures from global X-ray scattering data analysis of inverted hexagonal phases*
12.10 Barbara Eicher: *Curvature induced switching between transbilayer and intraleaflet coupling in asymmetric lipid vesicles*
12.30 Ryuta Ebihara: *Phase diagram of vesicle doublets*
12.50 Janez Štrancar: *Nanoparticle-driven translocation of epithelial membrane – missing link in NP-induced cardiovascular disease?*

13.10-15.00 Lunch

15.00-16.40 Cells and tissues (chair: Georg Pabst)

15.00 Maria Akhmanova: *Modeling of epithelial sheet deformation under external force applied by a migrating cell*
15.20 Bor Kavčič: *Translation bottlenecks and bacterial growth laws predict combined antibiotic action*
15.40 Jan Rozman: *3D vertex model of organoids and early embryos*
16.00 Antonio Šiber: *Topology of dividing planar tilings: Mitosis and ordering in epithelial tissues*
16.20 Saša Svetina: *Mechanism of red blood cell volume regulation based on the dependence of Piezo1 Ca^{++} permeability on membrane curvature*

16.40-17.10 Coffee break

17.10-18.20 Biopolymers II (chair: Tomislav Vuletić)

17.10 Mattia Marenda: *Molecular knots: Discovering privileged topologies with self-assembling models*
17.30 Kristina Serec: *Effect of magnesium ions on the structure of DNA thin films*
17.50 Andrea Papale: *Getting inspired by chromosome organization in eukaryotes: Ising model on polymers with complex topologies*

19.00-21.00 Dinner

21.00- Social event

Tuesday December 12 2017

8.00-9.00 Breakfast

9.00-10.20 New techniques and new technologies (chair: Saša Svetina)

9.00 Ida Delač Marion: *DNA tetrahedra and 2D materials hybrids*
9.20 Borna Radatović: *Process for forming ready-to-use QCM sensors with atomically flat surface suitable for scanning probe microscopies*
9.40 Lisa Marx: *Time-resolved X-ray studies of antimicrobial peptide activity in live E. coli on the nano- to micrometer scales*
10.00 Jure Derganc: *Passive migration of blood cells and lipid vesicles induced by concentration gradients in microcavities*
10.20 Jasmina Isaković: *The interactions of T-cell surface charge and electromagnetic fields generated around nodes of Ranvier in etiology of ischemic stroke and multiple sclerosis*

10.40-11.10 Coffee break

11.10-12.10 Colloids (chair: Antonio Šiber)

11.10 Clemens Jochum: *Equilibrium properties of DNA-dendrimers in electrolyte solutions*
11.30 Andreas-Kyriakos Doukas: *Liquid-drop model of polymeric nanocolloids at fluid-fluid interface*
11.50 Primož Ziherl: *Bronze-mean hexagonal quasicrystal*

12.30-14.00 Lunch

Departure

Abstracts

Modeling RNA interactions with SHAPE reagents

Vojtěch Mlýnský and Giovanni Bussi

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Function of RNA molecules usually depends on their global fold and on the presence of specific structural motifs. Chemical probing methods are routinely used in combination with nearest neighbor models to determine RNA secondary structure. In particular, selective 2'-hydroxyl acylation analyzed by primer extension (SHAPE) rapidly emerged as the gold standard method due to its capability to probe all RNA nucleotides [1] and the possibility to be used *in vivo* [2,3]. However, the structural determinants for SHAPE reactivity and its mechanism of reaction are still unclear. Here, molecular dynamics simulations and enhanced sampling techniques [4] are used to predict the accessibility of nucleotide analogs and larger RNA structural motifs to SHAPE reagents. We show that local RNA re-conformations are crucial in allowing reagents to reach 2'-OH group of a particular nucleotide, and that sugar pucker is a major structural factor influencing SHAPE reactivity [5]. The introduced protocol can be used for interpretation of previously unexplained reactivity patterns and provides the initial step for fast and cheap classification of alternating RNA structures.

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Simulations of supercoiled DNA rings

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DNA *in vivo* is constantly processed by the unceasing action of gyrases and other topoisomerase enzymes involved in replication, transcription and transpositions. In bacterial DNA, which is circular, the concurrent action of these enzymes introduces a significant amount of negative supercoiling as well complex forms of intra-molecular entanglements, particularly knots. As yet these two aspects have been mostly address separately: several studies have addressed how supercoiling constrains unknotted DNA rings and how knots affect torsionally-relaxed DNA. Only few investigations have considered simultaneously DNA supercoiling and knotting, and they were limited to the simplest topology, the trefoil knot, and to coarse-grained models with no explicit representation of the double-stranded chain. These considerations motivated us to consider topological constraints introduced by more complex knots, a 5_1 (torus) and 5_2 (twist) knot, in detailed models of 2 kbp-long DNA rings. These were described with the mesoscopic oxDNA model [1], which has an explicit representation of the double helix. I will report on the effect of the interplay of knotting and supercoiling on the dynamics and metric properties of such DNA rings.

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FCS testing of DNA interaction with cyclodextrine-based supramolecular systems functionalized with adamantyl guanidine

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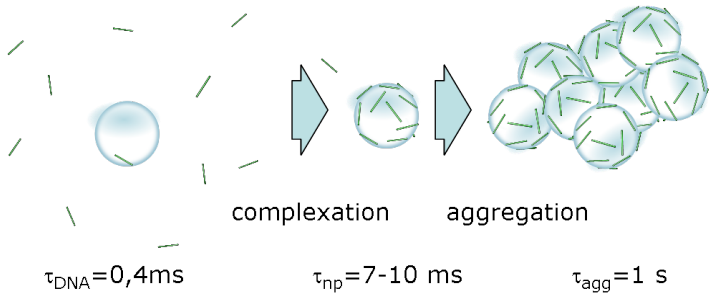
The aim of the present study was preparation of cyclodextrine based supramolecular systems functionalized with adamantyl guanidine and probing of their interaction with DNA using fluorescence correlation spectroscopy (FCS). We prepared and characterized supramolecular systems based on phosphatidylcholine liposome and vesicles of amphiphilic β-cyclodextrine (CD) derivative functionalized by entrapment of a series of adamantyl guanidines AG **1**-**5** [1,2]. Efficiency of incorporation of adamantyl guanidines into prepared supramolecular systems was measured spectrophotometrically, and the size and surface charge were determined by dynamic light scattering method. It was shown that all examined compounds were successfully incorporated into prepared supramolecular systems except compound AG**5**. The highest encapsulation efficiency was demonstrated for compound AG**1**. The incorporation of adamantyl guanidines did not affect the size of prepared vesicles but the vesicle charge was significantly changed. FCS was applied to examine the interactions between functionalized vesicles and the Cy5-fluorescently labelled, double-stranded, 120 bp DNA (DNA120*). The obtained results have clearly demonstrated that the vesicles with entrapped AG **1**-**4** present guanidinium groups on the surface of vesicles, which leads to interaction with DNA120* via guanidine-phosphate interaction. Also, it was shown that vesicles modified with adamantyl guanylhydrazones (AG **1**-**2**) bind DNA more efficiently, for almost an order of magnitude than vesicles modified with adamantyl aminoguanidines (AG **3**-**4**). Preliminary results have shown that prepared functional supramolecular systems strongly bind DNA and as such could be used in gene delivery.



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Conformational ensemble of an RNA hairpin: A combined maximum entropy and maximum parsimony approach

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An inverted SINEB2 (invSB2) element embedded in a non-coding RNA transcript has been identified as crucial for the enhancement of mRNA translation under cellular stress [1]. The transcript contains a sequence complementary to the target mRNA at its 5' end, and an invSB2 element at its 3' end, which performs the translation-enhancing function. A 29 nt RNA hairpin within invSB2 has been identified to be important for this process. Based on structural data (NOEs) from NMR experiments [2], the conformational ensemble of the hairpin was studied using molecular dynamics (MD) simulations with an enhanced sampling protocol with 8 replicas [3], while adaptive restraints according to the maximum entropy principle were applied to enforce agreement with the experimental data [4]. A cluster analysis based on the εRMSD, a metric that reports structural similarity in nucleic acids [5], and on the glycosidic bond angles yielded several conformational states. Averaging over the structures within one conformational cluster, it became evident that some NOEs are satisfied in specific clusters, while not in others, implying that the observed NOE signals represent a mixture of different conformations exchanging rapidly on a timescale below what can be resolved by NMR. We introduce a procedure that simultaneously maximizes the entropy of the resulting ensemble and minimizes the number of clusters involved, allowing us to represent the ensemble by a reduced number of significantly different structures. The loop motifs of the conformational clusters have been compared to RNA structures in the PDB database to learn more about possible functional mechanisms.

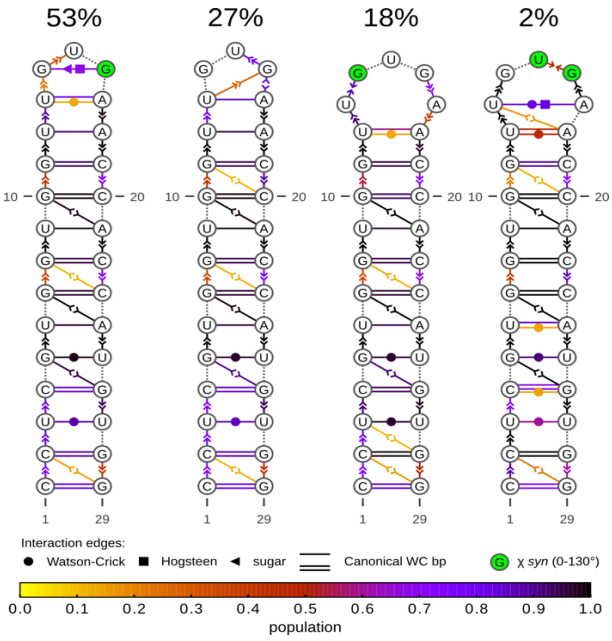

Figure 1: Minimal set of four conformations which agree with experimental data, with their respective predicted populations.

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Intrinsic lipid curvatures from global X-ray scattering data analysis of inverted hexagonal phases

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Intrinsic curvature J_0 is a property of lipids, which describes the bending radius of unstressed monolayers. It is an important parameter in the calculation of surface energies [1] and plays a substantial role in lipid/protein interactions [2]. We tested methods to measure J_0 with small-angle X-ray scattering (SAXS) experiments of inverted hexagonal phases (HII). The samples were prepared by the rapid solvent exchange-method and contained either the cone-shaped lipid dioleoyl phosphatidylethanolamine (DOPE) or mixtures of DOPE with diverse lamellar phase forming phosphatidylcholine lipids. Formerly used methods to evaluate the data included fitting the individual peaks to calculate the electron density profile, from which J_0 was deducted from the neutral plane position. Further, J_0's of non-HII forming lipids were determined by extrapolating the concentration dependent curvatures of their mixtures with DOPE [3]. In this work we explored a model-based approach for J_0 determination applying a full q-range SAXS data analysis. This approach would minimize the amount of samples required and also yield reliable intrinsic curvatures from weakly ordered H_{II} phases. Modelling included the calculation of the 2D-hexagonal structure factor and the electron density distribution within the lipid unit cell. The latter was described either in terms of the high-resolution scattering density profile [4], or low-resolution slab models, respectively. Additionally, modelling suggested the presence of a lipid monolayer, which coats the outer hydrophobic surface of the H_{II} aggregates. Both models for the electron density distribution as well as our previously developed method yielded comparable results for J_0. This favors the application of the slab model due to its lower number of adjustable parameters. The scattering density profile model in turn favors a joint analysis with neutron scattering data if more contrast is needed for data evaluation.

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Curvature-induced switching between transbilayer and intraleaflet coupling in asymmetric lipid vesicles

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We investigated the effect of intrinsic lipid curvature (J_0) on structural properties of asymmetric vesicles composed of palmitoyl-oleoyl-phosphatidylethanolamine (POPE; $J_0 < 0$), and palmitoyl-oleoyl-phosphatidylcholine (POPC; $J_0 \sim 0$). Cryo-electron microscopy and dynamic light scattering were used to evaluate vesicle size and morphology. Further, X-ray and neutron scattering combined with calorimetric measurements yielded insights into leaflet-specific lipid packing and melting processes. Strong transmembrane coupling in asymmetric vesicles with an inner leaflet composed of POPE and an outer leaflet enriched in POPC was observed below the lipid melting temperatures. This was shown by lipids melting cooperatively in both leaflets and a rearrangement of lipid packing in both leaflets. In contrast, no coupling was observed in vesicles with POPC inner bilayer leaflets and enriched POPE outer leaflets. In this case, the leaflets melted independently and did not affect each other's acyl chain packing. Additionally, no evidence for transbilayer coupling was found above the melting temperature of both systems regardless of the leaflet distribution of POPE. These findings are consistent with the energetically preferred location of POPE residing in the inner leaflet, where it is also located in natural membranes, most likely causing the coupling of both leaflets. The loss of this coupling in the fluid bilayers is probably the result of entropic contributions.

This work is supported by the Austrian Science Fund FWF, Project No. P27083-B20 (to G. P.).

Phase diagram of vesicle doublets

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We theoretically study the shape of vesicle doublets using the relaxed model where the total energy consists of the local bending term and the adhesion term and the reduced monolayer area difference is a free parameter. Using the Surface Evolver package, we numerically minimize the energy of doublets to find the stable doublets at various ratios of volumes of the two vesicles. We explore the phase diagram divided into (i) a region where vesicles are unbound, (ii) a region belonging to the axisymmetric doublets, which include cup-and-plug shapes in vesicles of very dissimilar volumes and macaron shapes in doublets consisting of vesicles of similar volumes, and (iii) a region containing nonaxsymmetric, sigmoid-shaped doublets. We analyze the nature of the phase transitions in detail and by evaluating the typical magnitude of the ADE terms, we estimate the range of parameters where the relaxed model is appropriate. The results are compared to our experimental studies of vesicle doublets and their transformations. We also present some results for vesicle aggregates containing more than two vesicles.

Nanoparticle-driven translocation of epithelial membrane – missing link in nanoparticle-induced cardiovascular disease?

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Although the link between nanoparticles (NPs) inhalation and cardiovascular disease has been identified a decade ago, the causal pathway leading to an increased activity of coagulation factors remains unknown. While coagulation occurs in blood, the two activating cofactors, the phosphatidylserine-containing membranes and tissue factor, are under normal conditions located in the epithelial cells on the other side of the air-blood barrier. Should NP be responsible for activation of the coagulation cascade, they will need to translocate alveolar cell membrane parts. To assess this novel hypothesis, we herein used advanced techniques such as Fluorescence Micro-Spectroscopy (FMS), Energy Dispersive Transmission Electron Microscopy (EDS TEM), super-resolution STED microscopy, and Fluorescence Correlation Spectroscopy (FCS). We clearly showed that NPs can impair the integrity of membranes and that such a disintegration is driven by the affinity between lipids and native NP surface. Finally, we – to our knowledge, for the first time – identified translocation of epithelial membrane driven by the NP-lipid interaction. The key missing link in the causal pathway leading to cardiovascular disease might therefore be a formation of mobile NP covered by epithelial plasma membrane , which can translocate membrane parts and potentially deliver activating cofactors into blood, finally leading to cardiovascular disease progression.

Modeling of epithelial sheet deformation under external force applied by a migrating cell

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Monolayered epithelium plays an important role in developing embryos, guiding tissue shape changes such as invagination, providing structural support and protection cover for inner tissues [1]. Theoretical studies showed how mechanical properties of epithelium on macroscopic and cellular levels are governing tissue deformations [2-4]. In the same time, acting as a barrier, epithelium interferes with cell spreading – process that is also crucial for development [5].

In the *Drosophila* embryo, immune cells migrate along the inner (basal) side of an epithelial layer during their invasion into the tail (Fig. 1a) [5,6]. They exert a force to separate two tissues and move forward (Fig. 1b). An *in vivo* pathway has been identified that lowers apical surface tension in the ectoderm of normal embryos to allow for sufficiently high speed of migrating cells. Knockout of its components leads to differential tension increase and impedes cell migration. We model out-of-plane epithelial deformation to derive how apparent stiffness of the sheet depends on its apical, lateral and basal tensions. Our study aims to understand how a mutual mechanical balance is achieved in tissues to allow for robust mechanical events, including cell migration.

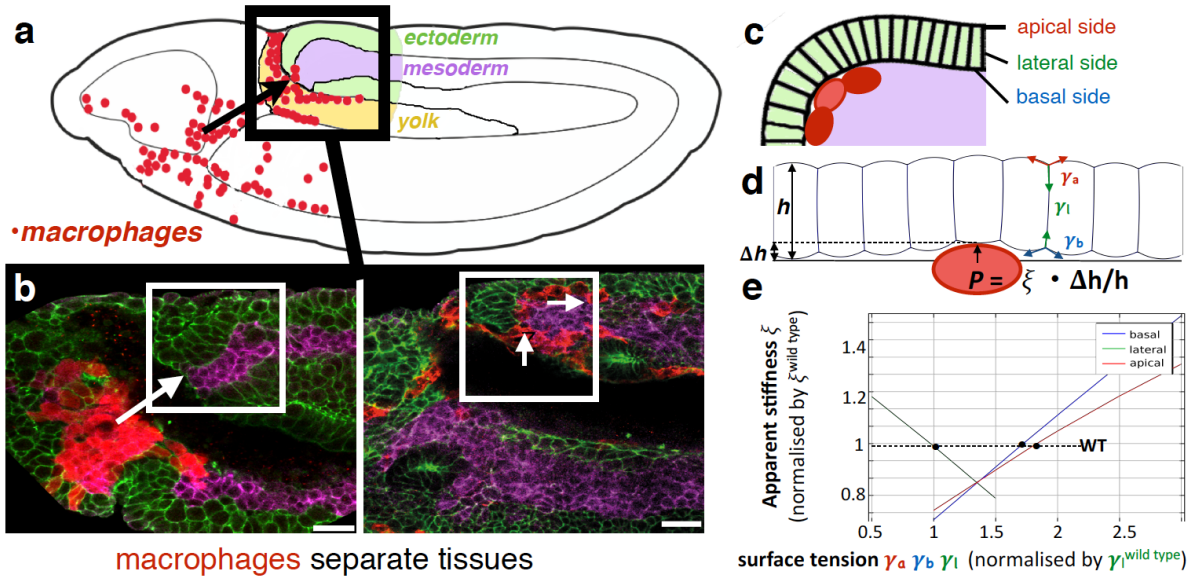

Figure 1: (a) Macrophages in Drosophila embryo encounter a tissue barrier on the way from the yolk into the germband. (b) They deform ectoderm and mesoderm tissues. (c) Ectoderm is a monolayered epithelium and can be described by a liquid-drop model (d) on long timescale (> 1 min). (e) Apparent stiffness of epithelium felt by a macrophage is proportional to apical and basal tensions and negatively proportional to the lateral tension.

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Translation bottlenecks and bacterial growth laws predict combined antibiotic action

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Fast growth of bacteria requires well-orchestrated translation machinery, which is modulated internally by translation factors and perturbed by certain antibiotics. The ability to predict the response of bacterial growth to single antibiotics, or to antibiotic combinations, would be of great fundamental and clinical significance. The effects of antibiotic combinations range from synergistic (inhibition is stronger) to antagonistic (inhibition is weaker) and have been hard to predict in the past, as the mechanisms underlying antibiotic interactions remain unknown. Here we hypothesize that the interactions between translation-inhibiting antibiotics result from kinetic properties of the antibiotics together with the interplay of different stages in which ribosomes are halted. To formalize this hypothesis, we developed a mathematical model that captures the following key processes: the kinetics of antibiotic binding to the ribosome, the synthesis of new ribosomes, effective dilution by growth, and up-regulation of ribosome synthesis upon inhibition of translation (as dictated by established growth laws). Despite the many processes involved, our model only depends on one key dimensionless parameter that can be estimated experimentally for individual antibiotics. To test model predictions, we selected several antibiotics that target translation and precisely measured their individual dose-response curves (the dependence of growth rate as a function of antibiotic concentration); from this, we predicted the dose-response surfaces (growth rate as a function over a two-dimensional gradient of antibiotic concentrations) for all their pairwise combinations, and compared them to direct measurements. To further improve our model, we examined how halting of the ribosomes in a specific stage affects the efficacy of antibiotics. We constructed bacterial strains in which we imposed artificial bottlenecks in translation by controlling the abundance of different translation factors using inducible promoters, and measured the antibiotic response of bacteria in the presence of such translation bottlenecks. These additional experiments, together with our mathematical model, allowed us for the first time to quantitatively predict interactions between pairs of antibiotics. Our findings offer new insights into the mechanisms of antibiotic interactions and translation itself and suggest a novel way of designing antibiotic therapies.

3D vertex model of organoids and early embryos

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We report a theoretical study of a fully 3D vertex-based model of an epithelium consisting of several hundred cells arranged around a yolk, with individual cells represented by prismatic or truncated-pyramid bodies carrying a certain surface tension on each functionally distinct face. We compute the shapes of the system for different values of the apical and basal tension, taking advantage of the fluidization of the epithelium due to active T1 topological transitions. We find that the shapes in different regions of the phase diagram correspond to two biologically distinct systems: Early embryos, which are often spherical or ellipsoidal in nature, and organoids, that is small shell-like aggregates of cells. We discuss the geometrical characterization of the shapes using their reduced volume and compare them to the physically somewhat similar system of vesicles.

Topology of dividing planar tilings: Mitosis and ordering in epithelial tissues

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Epithelial tissues can be well approximated as 2D polygon tilings of the plane. There are, however, infinitely many plane tilings, some ordered more than others and some seemingly "random", consisting of a range of polygon types and sizes. Not all tilings which can be imagined represent epithelial tissues, but those which do still represent a rather varied class, consisting of several subclasses. The tissues are, furthermore, dynamical tilings, as the cells they consist of divide [1]. The ordering of the epithelial tissue is thus, in general, a consequence of two effects: (i) energetics of cell-cell contacts and (ii) dynamical effects related to mitosis [2]. Here we concentrate on the second of the two effects and explore the stationary configurations of the tissues governed exclusively by the rules of cell division in which the energetics plays a secondary role, implicitly encoded in the rules. Depending on the rules chosen, three different epithelial classes are identified – a completely ordered tiling, consisting only of hexagons, a "random" tiling, consisting of many different polygons with comparable occurrence frequencies, and a semi-disordered tiling, consisting mainly of pentagons, hexagons and heptagons. The latter structure is often observed in real tissues [3].

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Mechanism of red blood cell volume regulation based on the dependence of Piezo1 Ca^{++} permeability on membrane curvature

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Red blood cell (RBC) can perform its primary function to carry respiratory gases also because of its ability to change its shape. RBC shape transformations can occur without much effort because its volume is much smaller than the volume of the sphere with the same membrane area and because of the flexibility of its membrane. Here we propose a mechanism of RBC volume regulation in which the regulated cell property is RBC reduced volume (i. e., the ratio between cell volume and its maximum possible volume). In the corresponding model it is assumed that RBC volume establishes through the regulation of the content of the RBC potassium. Potassium ions (K^+) are actively pumped into RBC by the sodium–potassium pump and are passively leaking out through several different channels. One of them is the Gardos channel which opens specifically for K^+ ions at increased RBC concentration of calcium ions (Ca^{++}). Ca^{++} ions can enter RBC under conditions which open the mechanosensitive Piezo1 channel [1]. Piezo1 structure [2] implies that fraction of open Piezo1 channels may also depend on membrane curvature and thus on the RBC shape. Curvature dependence of Piezo1 permeability is modeled by assuming that Piezo1 interacts with the surrounding membrane due to the mismatch between the intrinsic curvatures of the transmembrane part of this huge integral membrane protein and the principal curvatures of the membrane where it is located [3], and that Piezo1 intrinsic curvatures of its open conformation differ from that of its closed conformation. By also taking into account that RBC is in an osmotic equilibrium with the surrounding solution it is then possible to determine RBC reduced volume and its K^+ content. The consequent dependence of RBC volume on its membrane area is determined. The model explains why RBCs with higher than average membrane area have larger volumes and correspondingly RBCs with smaller areas smaller volumes [4]. The proposed mechanism for RBC volume regulation is further confirmed by the loss of this membrane area – cell volume correlation in RBC Piezo1 null mutation [1].

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Molecular knots:
Discovering privileged topologies with self-assembling models

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Molecular knots are increasingly studied not only for their ubiquity in biological contexts, but also for their distinctive geometrical features and peculiar mechanical behaviour. Reproducing, and harnessing, such properties in controlled contexts is one of the main objectives of synthetic chemistry where increasingly sophisticated techniques are used to guide the self-assembly of molecular building blocks into constructs with complex topologies [1]. Following our previous predictive investigation [2], we present here recent theoretical and computational results showing that schematic, coarse-grained models can help identify privileged topologies for self-assembling constructs. These are knot types that, owing to their geometry and symmetries are ideal target for supramolecular chemistry. The limited set of discovered topologies includes all knot types that have been successfully realised experimentally so far, as well as novel targets.

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Effect of magnesium ions on the structure of DNA thin films

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Interaction of the Mg^{+2} cations with DNA was previously studied by many authors as Mg ions show great affinity toward phosphate groups of DNA, thus neutralizing and stabilizing double helical structure [1-6]. However, due to great variety of experimental conditions, different authors report different affinities and preferable sites of Mg-DNA coordination, leaving particular mechanism of Mg-DNA interaction unclear.
In order to address how the behavior of DNA evolves upon progressive addition of Mg^{2+} cations, utilizing Fourier transform infrared spectroscopy, we have investigated vibrational properties of dsDNA thin films in a broad range of added magnesium chloride salt concentration. Also, to eliminate/determine influence of intrinsic sodium and magnesium ions, we have investigated both Na-DNA and Mg-DNA thin films where Mg-DNA was obtained by extensive dialysis towards respective $MgCl_2$ solutions.
Our results demonstrate that going from the low to the high magnesium content, cation–DNA interaction changes in strength due to enhanced Debye screening, present in the both the backbone as well as the base regions [7]. Whereas lower Mg^{2+} salt concentrations stabilize the double-helix B conformation of dsDNA, extremely high non-physiological contents, larger than 150 mM, induce fundamental modifications of the secondary structure, which possibly indicate a transition into a more compact form.

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Getting inspired by chromosome organization in eukaryotes: Ising model on polymers with complex topologies

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Each chromosome lies in the nucleus of eukaryotic cells and is made by a single filament of chromatin, a complex of DNA and proteins. Inside the nucleus, there exist regions where chromosomes condense into "territories" and others without chromatin ("interchromatin" compartments). Moreover, chromatin is not randomly distributed: in general, heterochromatin (a tightly packed form of chromatin which contains inactive genes) stays close to the nuclear periphery and euchromatin (a gene-rich, lightly packed form of chromatin) is concentrated toward the nuclear interior. Several models [1,2] use the state of chromatin as internal degree of freedom for polymers. I will discuss how to build an Ising model using different chromatin states on lattice polymers with complex topologies. These are inspired by bio-polymers [3] and can be mapped to real systems like chromosomes or supercoiled structures of DNA. In particular, I will show which of those model polymers exhibit a phase transition.

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DNA tetrahedra and 2D materials hybrids

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Compared to bulk material, interfaces exhibit additional rich physical phenomena. Functionalized surfaces represent interfaces which are of great importance not only in fundamental surface and materials science but also for applications. One implementation of functionalized surfaces are hybrid materials, as they bridge the gap between living matter and technology [1].

This work was focused on a study of two-dimensional (2D) materials that may template growth of the biomacromolecular layer, with the production of a hybrid structure as a final goal, which is defined as a layer of biomacromolecules on a suitable ordered substrate, with both systems having similar symmetry or distribution on a lateral scale: the hexagonal symmetry of the nanotemplated 2D material in combination with the DNA origami tetrahedral structure [2]. Two different 2D material templates were studied: either functionalized graphene or MoS_2, both on Ir(111) crystalline support. Graphene was grown directly on Ir(111) and subsequently functionalized with AuIr nanocluster array self-assembled onto a graphene moiré pattern. MoS_2 was grown on SiO_2 substrate and then transferred to Ir(111) [3]. Both template candidates were extensively characterized down to nanoscale, and their stability under ambient and in liquid conditions was confirmed. Taking into account the chemistry of the template materials (surfaces present either gold or sulphur), tetrahedron shaped DNA origami constructs with thiol-groups in three of the vertices were chosen as biomacromolecules of interest. Tetrahedra adsorption was calibrated on flat gold surfaces, and then applied to both 2D supports, thus producing two different hybrid systems, which were subsequently characterized. Such hybrid systems give promise for future applications in bio-optoelectronics as building blocks in various sensor chips, DNA microarrays, etc.

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Process for forming ready-to-use QCM sensors with atomically flat surface suitable for scanning probe microscopies

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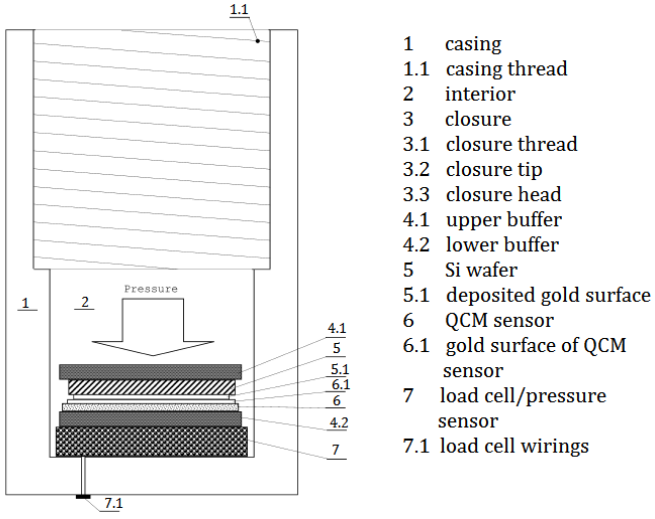
QCM (quartz micro balance) is a routinely used method in studies of biomacromolecular interactions with various substrates. It's application goes from biophysics, drug discovery, cell adhesion to new biomaterials and material science itself. As with any research tool, QCM is constantly upgraded and optimized in order to open new applications and new combinations with other techniques. [1]
One of the most attractive upgrades is combining scanning probe techniques like AFM (atomic force microscope) and STM (scanning tunneling microscope) in parallel with QCM, which would give for example not only information of total adsorption on surface, but also the information of exact placement of adsorption. To accomplish that, main challenge is producing ultra flat, functionalized surface of quartz chip that is used for QCM sensing – as the flatness is the key requirement for AFM and STM. [2]
Here we present our process for forming such a surface, essentially a modification of a regular, commercially available chip into a chip with atomically flat gold surface. We use a proprietary press. The press provides another advantage, as it protects this gold surface from adsorption of contaminants after preparation. We will present some AFM and STM studies that may utilize the flatness of this surface for imaging of biomacromolecules.



1 casing
1.1 casing thread
2 interior
3 closure
3.1 closure thread
3.2 closure tip
3.3 closure head
4.1 upper buffer
4.2 lower buffer
5 Si wafer
5.1 deposited gold surface
6 QCM sensor
6.1 gold surface of QCM sensor
7 load cell/pressure sensor
7.1 load cell wirings

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Time-resolved X-ray studies of antimicrobial peptide activity in live *E. coli* on the nano- to micrometer scales

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Infectious diseases caused by multi-resistant pathogenic bacteria are rapidly gaining grounds world-wide in health-care units. One highly promising strategy to combat infectious diseases is based on antimicrobial peptides (AMPs), effector molecules of innate immunity. Much of the biophysical insights about the molecular mode of action of AMPs relate to studies performed on lipid-only model systems. We performed time-resolved ultra-small angle X-ray scattering (USAXS) and SAXS experiments on live *Escherichia coli* (*E. coli*) under the attack of AMPS. These proof-of-principle experiments showed that changes induced by the peptides occur on the millisecond to second time scale, which is much faster than anticipated from previous experiments. Global analysis in terms of a multi core-shell model [1] demonstrated that most significant changes occur on the structural level of the inner and outer membrane of the bacteria. This demonstrates the feasibility of such studies and the ability to gain insight on rapid structural events on the nanometer scale in live systems, which will be further exploited to ultimately correlate time dependent changes on diverse levels of structural hierarchy in bacteria due to activity of AMPs.

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Passive migration of blood cells and lipid vesicles induced by concentration gradients in microcavities

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Passive migration of colloidal particles in concentration gradients is a relatively exotic phenomenon in colloidal science, first described in 1947 by Derjaguin and now broadly termed as *diffusiophoresis*. Here we report that diffusiophoresis can also affect blood cells and lipid vesicles.

In our experiments, cells and vesicles are placed into a flow-free environment in a microcavity extending from a simple microfluidic channel (Fig. 1A). When the solution in the main channel is exchanged by another solution of the same osmolarity, the solutes diffuse into and out from the cavity, causing transient concentration gradients that induce passive migration of cells and vesicles (Fig. 1B). Migration was observed in various electrolyte and non-electrolyte solutions with diverse solute diffusivities. Depending on the type of the exchanged solutions, the migration was directed towards the entrance or towards the end of the cavity, with migration distances up to several tens of micrometers. Diffusiophoresis can therefore significantly affect cell behavior in microcavities in biological and microfluidic systems.

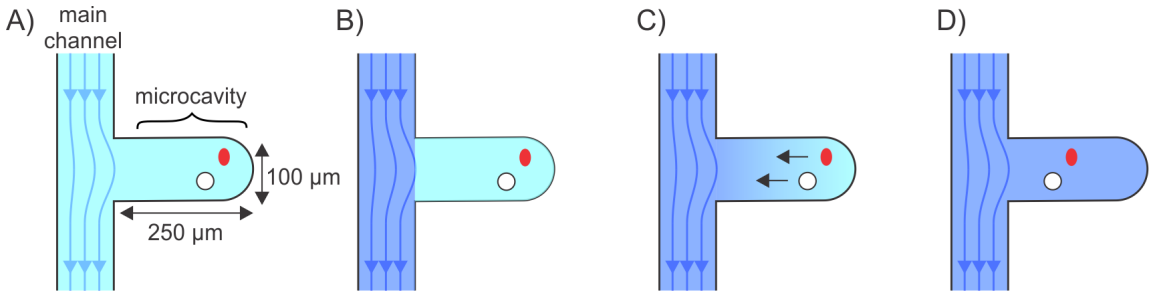

Figure 1: Schematic representation of the experimental protocol. A) Cells and vesicles are placed into a microcavity extending from the main microfluidic channel. The solution in the main channel flows by the cavity entrance while the back-end of the cavity remains flow-free. Cells and vesicles are transferred into the cavity by optical tweezers. B) The solution in the main channel (indicated in light blue) is exchanged by another solution of the same osmolarity (dark blue). C) The new solution diffuses into the cavity, and the old solution diffuses out of the cavity, causing transient concentration gradients of both solutes. Depending on the exchanged solutions, the cells and vesicles can migrate up or down the gradient. D) Migration stops when the cavity is filled with the new solution.

The interactions of T-cell surface charge and electromagnetic fields generated around nodes of Ranvier in etiology of ischemic stroke and multiple sclerosis

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This study utilized computational electromagnetics in Matlab and in-vivo SPION-enhanced MRI imaging to hypothesize that negative surface charge accumulated on a T-cells interacts with the electromagnetic fields generated around the nodes of Ranvier and thus initiates or mediates the autoimmune response in ischemic stroke and multiple sclerosis.

Since the total current flow through a neuron is the sum of the axial current from the previous neural segment and relevant ionic currents then, according to the Biot-Savart Law, a circular magnetic field should be generated around the neuron. According to Lorentz Force Law, this magnetic field then exerts a force on a moving charged particle, having the ability to deflect or attract the T-cell within the range of its radius. To test the hypothesis, T-cells were treated with Mifepristone (RU486), a glucocorticoid receptor antagonist shown to depolarize the T-cells, and then cortically injected into the left ventricle of mice with middle cerebral artery occlusion (MCAO). Superparamagnetic iron-oxide nanoparticles (SPION) were used as a visualizing agent for localization of T-cells and quantification of their mobility in the CNS.

Subsequent MRI scans showed that T-cells' mobility in CNS was impaired post-RU486 treatment. As opposed to the untreated T-cells in the positive control that migrated towards the MCAO lesion site, the T-cells treated with RU486 were stationary, at the cortical injection site, 1, 3, and 5 days post-injection. Further electromagnetic computational modeling quantified the temporal progression of the electromagnetic field around the nodes of Ranvier and its spatial distribution along a neuron to yield a numerical value for its strength and direction as well as proposed pathways of T-cell interaction with the electromagnetic field.

Leading off with the idea that untreated T-cells have a negative surface charge and can, therefore, interact with electromagnetic fields, this study suggests that impaired T-cell mobility post-glucocorticoid receptor antagonization is due to a depletion of external charge on a T-cell which, in turn, decreases its interaction with the electromagnetic fields generated around the nodes of Ranvier. This suggests that the electromagnetic fields around neurons and the innate electromagnetic properties of biological cells can can be utilized in producing biological materials that would depolarize or functionally neutralize T-cells, or designing coupled localized field-potentials that would reverse the innate electromagnetic fields in the CNS and alter the disease's course, be it multiple sclerosis or ischemic stroke.

Equilibrium properties of DNA-dendrimers in electrolyte solutions

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Dendrimers are synthetic macromolecules possessing a highly branched and regular internal structure. They are synthesized in a step-wise fashion by repeating units from various central multifunctional cores, on which radially branched shells called generations are covalently attached. Charging these dendrimers leads to conformational responsiveness, one of the most important ingredients for envisioned applications of the same, which is essentially lacking for their neutral counterparts.
Recently, Dan Luo and co-workers at Cornell University synthesized dendrimer-like DNA (DL-DNA) from the enzymatic ligation of Y-shaped DNA (Y-DNA) building blocks [1]. These charged DNA dendrimers are novel macromolecule aggregates, which hold high promise in bringing about targeted self-assembly of soft-matter systems in the bulk and at interfaces.
Inspired by these findings, we study systems of such DL-DNA molecules in order to advance the theoretical analysis of novel self-assembled structures. First, we simulate a single DL-DNA molecule, whose base-pairs are modeled by charged monomers. Their interactions are chosen to mimic the equilibrium properties of DNA correctly. We then employ MD simulations to measure the dependence of equilibrium properties, e.g. the influence of salinity, the tensor of gyration, and form factors, on the dendrimer's generation.
The obtained results are compared to experiments. In the future, we plan to use DL-DNA to investigate the phenomenon of cluster crystals in the bulk [2], a novel form of solids with multiple site occupancy. Furthermore, we want to study two-dimensional surface ordering of low-generation DL-DNA and Y-DNA with tunable rigidity around the junction point [3].
The study of these charged dendrimer-systems is an important field of research in the area of soft matter due to their potential role to various interdisciplinary applications [4, 5], ranging from molecular cages and carriers for drug and gene delivery in a living organism to the development of dendrimer/dendron-based ultra-thin films (monolayers and multilayers) in the area of nanotechnology.

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Liquid-drop model of polymeric nanocolloids at fluid-fluid interface

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We theoretically study the structure of a monolayer of soft nanocolloidal particles trapped at a fluid-fluid interface [1]. We use a coarse-grained representation where the particles are modeled as liquid drops characterized by a given reference volume and compressibility as well as two drop-fluid surface tensions and one drop-drop interfacial tension [2]. The presence of the fluid-fluid interface results in a non-spherical, lens-like resting drop shape. We compute the free energy of a crystalline monolayer for several trial 2D lattices, and we construct the equilibrium phase diagram of this quasi-2D system. We find two distinct mechanisms that result in a non-convex free energy, which in turn translates into an isostructural phase transition. At very low drop compressibility, we observe that the formation of contact zones between nominally attractive drops does not take place at the smallest density where the drops touch but only at a larger density, which happens due to the presence of the fluid-fluid interface. We compare our theoretical results such as the pressure-area isotherms to a recent experimental study of core-shell microgel particles [3], and we find good agreement for several combinations of the model parameters.

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Bronze-mean hexagonal quasicrystal

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The most striking feature of conventional quasicrystals is their non-traditional symmetry characterized by icosahedral, dodecagonal, decagonal or octagonal axes. The symmetry and the aperiodicity of these materials stem from an irrational ratio of two or more length scales controlling their structure, the best-known examples being the Penrose and the Ammann–Beenker tiling as two-dimensional models related to the golden and the silver mean, respectively. Surprisingly, no other metallic-mean tilings have been discovered so far. Here we propose a self-similar bronze-mean hexagonal pattern, which may be viewed as a projection of a higher-dimensional periodic lattice with a Koch-like snowflake projection window. We use numerical simulations to demonstrate that a disordered variant of this quasicrystal can be materialized in soft polymeric colloidal particles with a core–shell architecture. Moreover, by varying the geometry of the pattern we generate a continuous sequence of structures, which provide an alternative interpretation of quasicrystalline approximants observed in several metal–silicon alloys.