9th Christmas Biophysics workshop

XBW2014

Book of abstracts

Hotel Vela Vrata, Buzet, Croatia
15.-16. December 2014.

Croatian Biophysical Society, December 2014.
www.biofizika.hr

Christmas Biophysics Workshops are annual scientific meetings of regional research groups from Slovenia, Croatia, Austria and Italy in the fields of biophysics, soft matter physics, and closely related fields. The workshop series were initiated in 2006 by Silvia Tomić (Zagreb) and Rudolf Podgornik (Ljubljana). Here direct contacts, research plans and friendships can be established or maintained in a relaxed atmosphere, just before Christmas.

Scientific committee:

Antonio Šiber

Tomislav Vuletić

Organizing committee:

Sanjin Marion

Ida Delač Marion

This Workshop was supported by:

Croatian Biophysical Society

Croatian Ministry of Science, Education and Sports

XBW2014 Monday, 15^{th} December

9:00–10:00	**Arrival and registration**	
10:00-10:10	**Opening word (Antonio Šiber and Tomislav Vuletić)**	

DNA (Chair: Nenad Pavin)

10:10	**Ida Delač Marion**	*Polyelectrolyte composite: Hyaluronic acid mixture with DNA*
10:30	**Danijel Grgičin**	*A dynamics study of a structural problem: DNA melting studied by electrical transport*
10:50	**Antonio Suma**	*Knotting and Unknotting Dynamics of DNA Strands in Nanochannels*
11:10	**Sanjin Marion**	*DNA with condensing proteins in confinement*
11:30–12:00	**Coffee Break**	

Membranes I (Chair: Primož Ziherl)

12:00	**Mihal Belička**	*Polar headgroup dependence of the unilamellar vesicles structure obtained by SANS*
12:20	**Peter Heftberger**	*Influence of domain size on structure and elastic fluctuations in complex lipid mixtures*
12:40	**Benjamin Kollmitzer**	*Membrane domain interactions by Monte Carlo type analysis of osmotic stress data*
13:00	**Iztok Urbančić**	*Resolving Internal Motional Correlations Completes the Conformational Entropy Meter*
13.30-15.00	**Lunch**	

Soft matter (Chair: Tomislav Vuletić)

15:10	**Guido Polles**	*Optimizing the self-assembly of knotted constructs by tuning the building blocks geometry*
15:30	**Primož Ziherl**	*Antinematic local order in dendrimer liquids*
15:50	**Uroš Tkalec**	*Tunable nematic liquid crystal flows in microfluidic confinement*
16:10	**Luca Ponzoni**	*Quasi-rigid domains of proteins identified via dimensional reduction of distance fluctuation matrices*
16:30–17:10	**Coffee Break**	

Physics of Cells and Tissues (Chair: Antonio Šiber)

17:10	**Nadica Ivošević DeNardis**	*Kinetics of adhesion and spreading of living cell at the charged interface*
17:30	**Matej Krajnc**	*Surface tension-based mechanics of epithelia*
17:50	**Nenad Pavin**	*Forces balance in the mitotic spindle*
18:10	**Marcel Prelogović**	*Cross-linking proteins facilitate formation of microtubule bundles*
19:00–20:30	**Dinner**	
20:30–	**Social event**	

XBW2014 Tuesday, 16^{th} December

7:30–8:45	**Breakfast**	

From Nano to Bio (Chair: Christian Micheletti)

9:00	**Martina Lihter**	*Nanopores in SiN_x membranes*
9:20	**Ke Liu**	*2D Nanopores from Graphene to Molybdenum Disulfide*
9:40	**Ivana Nikić**	*Investigation of molecular ligand-receptor recognition tuned by cryoprotectants*
10:00	**Atiđa Selmani**	*Role of the pH and electrolyte on the photocatalysis efficiency of the TiO_2 one dimensional nanomaterials*
10:20	**Janez Štrancar**	*Lipid bilayer explosion driven by titan-oxide nanoparticles*
10:40–11:20	**Coffee Break**	

Membranes II (Chair: Georg Pabst)

11:20	**Bojan Božič**	*The behavior of the tension pore induced by a pore-forming agent*
11:40	**Bing-Sui Lu**	*Fluctuation pressure of a membrane subject to hard wall constraints: a self-consistent approach*
12:00	**Suzana Šegota**	*Charged Amphiphylic Ligands of Nanoparticles Increase Lateral Compaction of Membranes. Nanomechanical and Thermotropic Study of Model Lipid Membranes in High Ionic Strength Solutions*
12:20	**Urška Jelerčič**	*Pearling instability of membrane tubes driven by curved proteins and actin polymerisation*
12:40	**Markus Miettinen**	*Open collaboration that uses NMR data to judge the correctness of phospholipid glycerol and head group structures in molecular dynamics simulations*
13:00	**Closing remarks**	
13:30–15:00	**Lunch**	
15:00–	**Departure**	

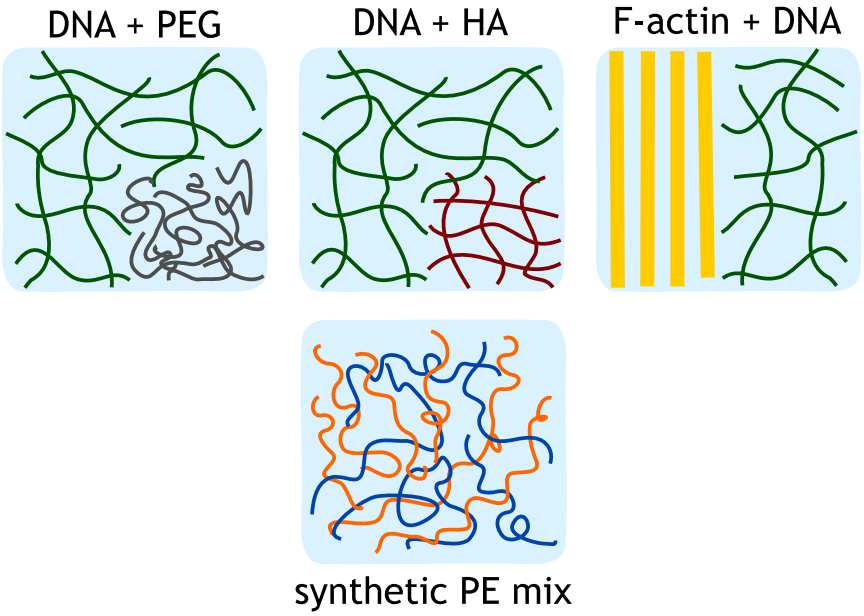
10:10
DNA

Polyelectrolyte composite: Hyaluronic acid mixture with DNA

I. Delač Marion[1*], D. Grgičin[1], K. Salamon[1], S. Bernstorff[2], and T. Vuletić[1]

1 Institut za fiziku, Bijenička 46, 10000 Zagreb, Croatia
2 Elettra-Sincrotrone Trieste, 34149 Basovizza, Italy
** idelac@ifs.hr*

We studied salt-free, highly concentrated (5-200 g/L) mixtures of unfragmented (μm contour length) DNA and hyaluronic acid (HA) as a border-line example of rigid-rod/flexible-chain composite, across a broad range of concentration ratios $c_{HA}/c_{DNA} = 0.05 - 50$. By polarizing microscopy (PM) we established that the DNA and HA form clearly separated thread-like domains defined and oriented by solution shear. Within its domains DNA shows birefringent banded patterns, routinely observed for long chain mesogens. We applied small angle x-ray scattering (SAXS) to the mixtures and observed a PE correlation peak at $q^\star$ wave vector. This peak was ascribed to DNA subphase and was used as a measure of effective DNA concentration in the subphase, according to deGennes scaling relationship between the DNA mesh size $\xi = 2\pi/q^\star \approx c^{-1/2}$ and monomer concentration c[1]. From c_{DNA} we inferred the effective c_{HA} of HA subphase, and found a proportionality $c_{HA} = 0.8 c_{DNA}$. As DNA and HA subphases are in the osmotic pressure equilibrium, HA osmotic pressure $\Pi_{HA} = \Pi_{DNA}$ is inferred, since the DNA equation of state is known. That is, $\Pi_{HA}(c)$ scales as for the other PEs (DNA and polystyrene sulfonate, PSS), $\Pi \sim c^{9/8}$, up to about $c = 1$ M. The osmotic pressure of PEs is regulated by Manning uncondensed counterion concentrations, $c_i/c = \phi < 1$. Since HA, a weak PE due to a low linear charge, does not feature condensation, i.e. $c_i = c$, it may be used as a measure of counterion concetrations for strong PEs. Eventually, we corroborate the work by Raspaud et al. [2] who found that the concentration of counterions controlling the osmotic pressure is double the theoretical Manning-condensation defined value for DNA or PSS.



[1] *K. Salamon,D. Aumiler, G. Pabst, T. Vuletić (2013) Probing the Mesh Formed by the Semirigid Polyelectrolytes* Macromolecules *46:1107–1118.*

[2] *E. Raspaud,M. da Conceiçao, F. Livolant (2000) Do Free DNA Counterions Control the Osmotic Pressure?* Phys. Rev. Lett. *84:2533–2536.*

A dynamics study of a structural problem: DNA melting studied by electrical transport

10:30
DNA

D. Grgičin[1*], D. Vurnek[2], T. Vuletić[1]

1 Institut za fiziku, Bijenička cesta 46, 10000 Zagreb, Croatia
2 Institute for Theoretical Physics I, FAU, Erlangen
** dgrgicin@ifs.hr*

DNA melting has been studied by UV-spectrophotometry (UVS) since 1970's [1]. The effects of base stacking and hydrogen bonds between the complementary bases keep the double stranded (dsDNA) configuration, while Coulomb repulsion of phosphate groups destabilizes DNA and may separate it into two strands (ssDNA). The melting temperature dependence on DNA sequence/composition/size, DNA and added salt concentration and counterion species/valence has been established. We report a comprehensive study how conductometry and impedance spectroscopy reflect the DNA conformation and counterion atmosphere dependence on these variables. We studied short DNA (150 basepairs, bp), dilute solutions as well as very long (2-100 kbp) DNA, semidilute solutions (DNA 0.003-10mM), with Na^+ or Mg^{++} counterions (NaDNA and MgDNA), with and without added salt (0.1-1 mM NaCl, $MgCl_2$). The applied techniques have been used to get the two parameters to describe a polyelectrolyte [2, 3]. The de Gennes correlation length (or the polyion mesh size) ξ describes the polyion subsystem and the Manning free counterions fraction θ describes the counterion distribution around the polyion. From conductometry we extract the values for θ that are in accord with Manning theory [4] both for NaDNA and MgDNA above 1mM. Further we studied the increase of θ towards lower DNA concentrations. It is in theory related to the entropic gain that occurs only for finite sized polyions upon reduction in concentration [5]. However, we observe this both for short and long DNA and expectedly not if the salt was added - presence of salt suppresses the gain in entropy upon decondensation. The decondensation increases the Coulomb repulsion of DNA strands and leads to DNA melting that we observe as a strong increase in the molar conductivity, above the effects of decondensation. This is due to ssDNA having a higher θ compared to dsDNA. Indeed we found this for NaDNA but not for MgDNA which is known to be more stable from UVS. We are attempting to reconcile these findings with the impedance spectroscopy which provides a measure of ξ dependence for long DNA. The ξ vs. c indicates denaturation of NaDNA and the absence of it for MgDNA - indicatively, at the same concentrations as found by conductometry. [2, 6, 7].

[1] M. T. Record Jr., Biopolymers **14**, *2137 (1975).*

[2] T. Vuletić, S. Dolanski Babić, D. Grgičin, D. Aumiler, J. Raedler, F. Livolant, S. Tomić, Phys. Rev. E **83**, *041803 (2011).*

[3] C. Wandrey, D. Hunkeler, U. Wendler, W. Jaeger, Macromolecules **33**, *7136 (2000).*

[4] G. S. Manning, Quart.Rev.Biophys. **11**, *179, (1978).*

[5] D. Antypov and C. Holm, Phys. Rev. Lett. **96**, *088302 (2006).*

[6] K. Salamon, D. Aumiler, G. Pabst, T. Vuletić, Macromolecules, **46**, *1107 (2013).*

[7] D. Grgičin, S. Dolanski Babić, T. Ivek, S. Tomić and R. Podgornik, Phys. Rev. E **88**, *052703 (2013).*

10:50 DNA

Knotting and Unknotting Dynamics of DNA Strands in Nanochannels

A. Suma[1], E. Orlandini[2], C. Micheletti[1]

1 SISSA, International School for Advanced Studies, via Bonomea 265, I-34136 Trieste, Italy
2 Dipartimento di Fisica, Sezione CNISM, and Università di Padova, via Marzolo 8, I-35131 Padova, Italy

The self-knotting dynamics of DNA strands confined in nanochannels can affect its metric and mechanical properties, and interfere with the elongation process in nanofluidics devices. We characterize, through Brownian simulations, how the knotted states arise from the internal dynamics of the chain and show that it is possibile to recover the well-characterized equilibrium knotting probability. In Ref.[1], the behaviour for model DNA chains of 3.6 μm is studied inside channels 50-300 nm wide, covering the transition between different metric scaling regimes and the concomitant drop of DNA knotting probability for channel widths below $\sim$ 75 nm . It is found that knots typically originate from deep looping and back-foldings of the chain ends, and upon lowering the channel width, backfoldings become shallower and rarer and the lifetime of knots decreases while that of unknots increases. Following this results, we restrict ourselves to channel width of 56 nm, where the bakfolding, and so the knotting became rarer, and vary the length of the chain from 1.2 to 4.8 nm, analyzing how the topological and knotting properties vary increasing the length. The results can aid the design of nanochannels capable of harnessing the self-knotting dynamics to quench or relax the DNA topological state as desired.

[1] C. Micheletti, E. Orlandini (2014) Knotting and Unknotting Dynamics of DNA Strands in Nanochannels. ACS Macro Lett. *3 (9), 876–880.*

DNA with condensing proteins in confinement

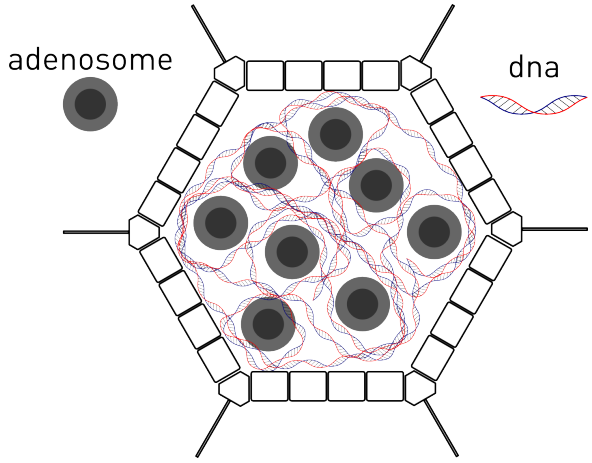
11:10
DNA

Sanjin Marion[1], Ana J. Perez Berna[2], Carmen San Martin[2], Antonio Šiber[1]

1 Institute of Physics, Bijenička cesta 46, HR-10000 Zagreb, Croatia
2 Department of Macromolecular Structure, Centro Nacional de Biotecnologia (CNB-CSIC), Darwin 3, 28049 Madrid,Spain

Nature has found various ways to pack DNA into small spaces. A well known example is the packing of DNA in chromosomes where highly basic histone proteins wrap the DNA, forming thus protein-DNA complexes called *nucleosomes* which can be more easily fitted in small volume. Similar packing mechanisms have been found in adenoviruses where DNA-condensing proteins encoded in the viral genome condense the DNA in the capsid[1]. This is an unusual device in the world of DNA viruses. Packing of DNA in adenoviruses has long evaded precise description since the viral DNA molecule condensed by proteins (core) lacks icosahedral order characteristic of the virus protein coating (capsid)[3]. Still, the dominant view is that the core has an ordered structure.

We show that useful insights regarding the organization of the core can be inferred from the analysis of spatial distributions of the condensing proteins. These were obtained from the inspection of contrast in cryo-EM cross-sections of mature and immature adenoviruses. Our analysis shows that the core lacks symmetry and strict order, yet the distribution of the condensing proteins is not entirely random. Comparisons between mature and immature virions showed no visible differences. The features of the distribution can be explained by modelling the condensing proteins and the part of the DNA each of them binds as very soft spheres, interacting repulsively with each other and with the capsid. Results show that a backbone of DNA linking the condensing proteins is not needed to explain the experimental results. Although these condensing proteins are connected by DNA in disrupted virion cores, the in vivo capsid is a crowded environment which changes the effective interactions involved in the packing of the DNA material[4].



[1] Carmen San Martín. Latest insights on adenovirus structure and assembly. Viruses *(2012), 4(5):847–77.*

[2] Antonio Siber, Anže Lošdorfer Božič, and Rudolf Podgornik. Energies and pressures in viruses: contribution of nonspecific electrostatic interactions. Phys. Chem. Chem. Phys. *(2012), 14(11):3746–65.*

[3] Ana J Pérez-Berná, Roberto Marabini, Sjors H W Scheres, Rosa Menéndez-Conejero, Igor P Dmitriev, David T Curiel, Walter F Mangel, S Jane Flint, and Carmen San Martín. Structure and uncoating of immature adenovirus. J. Mol. Biol. *(2009), 392(2):547–57.*

[4] A.P. Minton. Influence of excluded volume upon macromolecular structure and associations in 'crowded' media. Curr. Opin. Biotechnol. *(1997), 8(1):65–9.*

12:00
M1

Polar headgroup dependence of the unilamellar vesicles structure obtained by SANS

M. Beličkа[1*], M. Klacsová[2], J. Teixeira[3], P. Balgavý[2]

1 Institute of Molecular Biosciences, Biophysics Division, University of Graz, Graz, Austria
2 Faculty of Pharmacy, Comenius University, Bratislava, Slovakia
3 Laboratoire Leon Brillouin, CEA, Saclay, France
** michal.belicka@uni-graz.at*

The measurements of small-angle neutron scattering (SANS) were performed on unilamellar vesicles formed by the mixtures of 1-palmitoyl-2-oleoyl-*sn*-glycero-3-phosphatidylethanolamine (POPE), 1-palmitoyl-2-oleoyl-*sn*-glycero-3-phosphatidylcholine (POPC) and 1-palmitoyl-2-oleoyl-*sn*-glycero-3-phosphatidylserine (POPS). The molar ratios of POPC and POPE in lipid bilayers were mutually changed in the range from 0 to 96 molar percent. This allowed to effectively change the average volume of the lipid polar head with only minor change of its structure, while keeping the composition of lipid hydrocarbon chains region unchanged. For the description of internal structure of lipid bilayer we used 3-strip model describing hydrophilic and hydrophobic environments of bilayer as homogeneous regions. The obtained results show ideal mixing of the lipids inside bilayers in all prepared samples. Albeit POPC differs from POPE only in the terminal choline methyl groups, the corresponding change in the polar headgroup volume influences lateral area per lipid molecule significantly. We found that the decrease in the average polar headgroup volume is directly connected with the decrease in the area per lipid molecule and, therefore, also with increase in the bilayer hydrophobic core thickness.

Influence of domain size on structure and elastic fluctuations in complex lipid mixtures

12:20
M1

P. Heftberger[1], B. Kollmitzer[1], A. Rieder[1], G. Pabst[1*]

1 University of Graz, Institute of Molecular Biosciences, Biophysics Division, NAWI Graz, Humboldstr. 50/III, A-8010 Graz, Austria
** georg.pabst@uni-graz.at*

Lipid-only domains are well-established mimetic systems for membrane rafts enabling the study of their physical properties under strictly controlled conditions. Of particular interest are four component lipid mixtures entailing the variation of lipid domain size from micron regime down to a few nanometers [1]. Applying our recently developed small-angle x-ray scattering data analysis technique, we have studied changes of membrane thickness, lateral lipid packing and bending fluctuations for coexisting liquid-ordered (Lo) and liquid-disordered (Ld) phases in DOPC/POPC/DSPC/cholesterol mixtures along this domain-size trajectory, including the melting of Lo domains as a function of temperature. Bending fluctuations for coexisting Lo domains were found to be significantly lower than for single Lo phases at the boundary of the Lo+Ld regime. In turn, little variation was observed when domains exceeded sizes of 160 nm. Further, we found that the melting of Lo domains as a function of temperature is controlled by thickness differences between Lo and Ld and the associated domain line tension.

This work was supported by Austrian Science Fund FWF, Project No. P24459-B20.

[1] F.A. Heberle et al. (2013) J. Am. Chem. Soc. 135 (18) *6853-6859.*

12:40 M1

Membrane domain interactions by Monte Carlo type analysis of osmotic stress data

B. Kollmitzer[1,2*], P. Heftberger[1,2], H. Amenitsch[3], R. Podgornik[4,5], J.F. Nagle[6], G. Pabst[1,2]

1 Institute of Molecular Biosciences, Biophysics Division, University of Graz, NAWI Graz, Austria
2 BioTechMed-Graz, Austria
3 Institute of Inorganic Chemistry, Graz University of Technology, Graz, Austria
4 Department of Theoretical Physics, Jozef Stefan Institute and Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia
5 Department of Physics, University of Massachusetts, Amherst, Massachusetts, USA
6 Department of Physics, Carnegie Mellon University, Pittsburgh, Pennsylvania, USA
** Benjamin.Kollmitzer@uni-graz.at*

Diverse physiological processes in living systems depend on fundamental interactions of physical origin on the nanoscopic length scale. Of particular interest are forces acting between membrane domains/rafts across the aqueous phase governing their mutual alignment. Besides bare interactions, such as van der Waals attraction or solvation (hydration) forces, also membrane bending fluctuations, which relate to domains' bending rigidities, need to be considered. We have developed a method based on Monte Carlo simulations and global small-angle X-ray scattering analysis, allowing us to scrutinize osmotic stress data of coexisting liquid-ordered (Lo)/ liquid-disordered (Ld) domains for interdomain interactions. We report results for DSPC/DOPC/cholesterol and DPPC/DOPC/cholesterol lipid mixtures and focus in particular on the bending rigidities of Lo/Ld phases. Results are discussed with respect to effects on membrane-mediated partitioning of proteins in different lipid environments, domain line-tension and size-dependent alignment of like-domains.

This work is supported by the Austrian Science Funds FWF, Project No. P24459.

13:00
M1

Resolving Internal Motional Correlations Completes the Conformational Entropy Meter

I. Urbančič, A. Ljubetič, J. Štrancar*

Laboratory of Biophysics, Condensed Matter Physics Department, "Jožef Stefan" Institute, Jamova cesta 39, SI-1000 Ljubljana, Slovenia
** janez.strancar@ijs.si*

Conformational entropy (S_Ω) has long been used to theoretically characterize the dynamics of proteins, DNA, and other polymers. Though recent advances enabled its calculation also from simulations and nuclear magnetic resonance (NMR) relaxation experiments[1], correlated molecular motion has hitherto greatly hindered both numerical and experimental determination, requiring demanding empirical and computational calibrations. We have recently shown that these motional correlations can be estimated directly from temperature-dependent S_Ω data that reveal effective persistence lengths of the polymers (Figure 1), which we demonstrated by measuring S_Ω of amphiphilic molecules in model lipid systems by spin-labeling electron paramagnetic resonance (EPR) spectroscopy[2]. We validated our correlation-corrected S_Ω meter against the basic biophysical interactions underlying biomembrane formation and stability (Figure 2), against the changes in enthalpy and diffusion coefficients upon phase transitions, and against the energetics of fatty acid dissociation. As the method can be directly applied to conformational analysis of proteins and other polymers, as well as adapted to NMR or polarized fluorescence techniques, we believe that the approach can greatly enrich the scope of experimentally available statistical thermodynamics, offering new physical insights into the behavior of biomolecules.

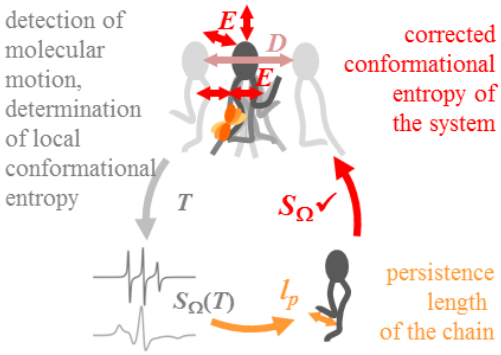


Fig. 1 Schematic description of the method to determine conformational entropy of molecules, corrected for the correlations of internal motion, by EPR spectroscopy.

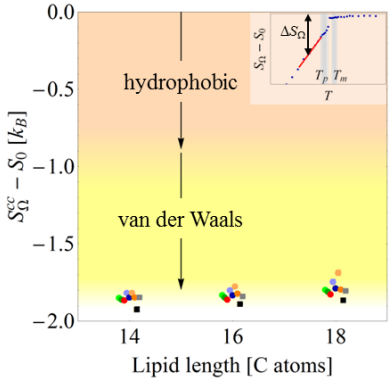


Fig 2 Conformational entropies, measured by various spin labels (colored symbols) in different model membranes in gel phase, are compared to the two main energetic contributions.

[1] M. S. Marlow, J. Dogan, K. K. Frederick, K. G. Valentine, and A. J. Wand (2010) Nat. Chem. Biol. *6, 352.*

[2] I. Urbančič, A. Ljubetič, and J. Štrancar (2014) J. Phys. Chem. Lett. *5, 3593.*

15:10 SM

Optimizing the self-assembly of knotted constructs by tuning the building blocks geometry

G. Polles[1], D. Marenduzzo[1], E. Orlandini[2], C. Micheletti[1,3*]

1 SISSA, International School for Advanced Studies, via Bonomea 265, I-34136 Trieste, Italy
2 SUPA, School of Physics, University of Edinburgh, Mayfield Road, Edinburgh EH9 3JZ, Scotland
3 Dipartimento di Fisica e Astronomia and Sezione INFN, Universitá di Padova, Via Marzolo 8, 35131 Padova, Italy

Self-assembling systems are a field of growing interest in physics because of their ability to form complex machineries or materials from relatively simple building blocks. We performed an in silico study regarding the possibility to designing the geometry of monodispersed building blocks with attractive ends so that they can assemble in three-dimensional structures of non-trivial topology.

We show that blocks of different geometry one can form constructs tied in different types of knots.

We conclude that the building blocks shape can be tuned to direct the spontaneous assembly towards well defined and knotted shapes.

Antinematic local order in dendrimer liquids

15:30
SM

I. A. Georgiou[1], P. Ziherl[2,3,*] and G. Kahl[4]

1 Institute for Theoretical Physics, Technische Universität Wien, Wiedner Hauptstrasse 8-10, A-1040 Vienna, Austria
2 Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia
3 Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia
4 Institute for Theoretical Physics and Center for Computational Materials Science, Technische Universität Wien, Wiedner Hauptstrasse 8-10, A-1040 Vienna, Austria
** primoz.ziherl@ijs.si*

We use monomer-resolved numerical simulations to study the positional and orientational structure of a dense dendrimer solution, focusing on the effects of the prolate shape and deformability of the dendrimers on the short-range order. Our results provide unambiguous evidence that the nearest-neighbor shell of a tagged particle consists of a mixture of crossed, side-by-side, side-to-end, and end-to-end pair configurations, imposing antinematic rather than nematic order observed in undeformable rodlike particles. This packing pattern persists even at densities where particle overlap becomes sizable. We demonstrate that the antinematic arrangement is compatible with the A15 crystal lattice reported in several dendrimer compounds [1].

[1] I. A. Georgiou, P. Ziherl, and G. Kahl, (2014) Antinematic local order in dendrimer liquids EPL *106:44004*

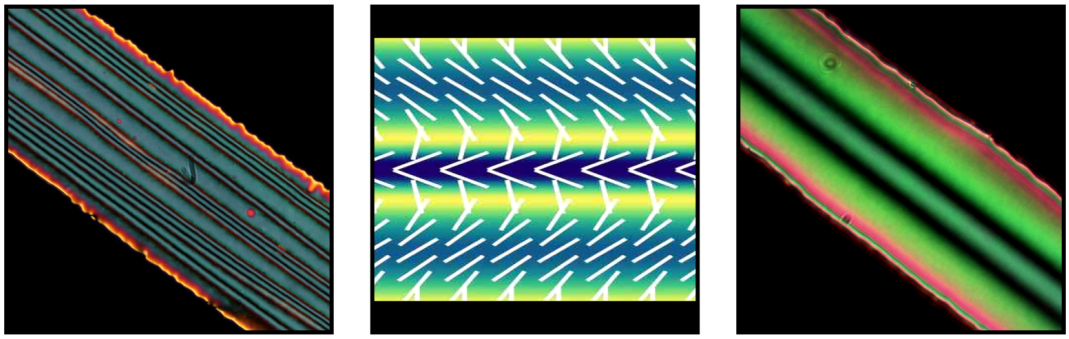
15:50 SM

Tunable nematic liquid crystal flows in microfluidic confinement

U. Tkalec[1,2,3*], A. Sengupta[4,5], M. Ravnik[6], C. Bahr[4], S. Herminghaus[4]

[1] *Institute of Biophysics, Faculty of Medicine, University of Ljubljana, Slovenia*
[2] *Faculty of Natural Sciences and Mathematics, University of Maribor, Slovenia*
[3] *Jožef Stefan Institute, Ljubljana, Slovenia*
[4] *Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany*
[5] *Massachusetts Institute of Technology, Cambridge, U.S.A.*
[6] *Faculty of Mathematics and Physics, Ljubljana, Slovenia*
* *uros.tkalec@ijs.si*

Flow of a nematic liquid crystal on a micro-scale is complex due to the inherent coupling between the material flow and the long-range orientational order of an anisotropic fluid. This coupling offers sensitive driving mechanism for controlling the liquid crystal flow in conventional microfluidic setups. We present experimental studies of passive nematic flow in microchannels with homeotropic surface anchoring conditions. We show how different characteristic flow regimes depend on the driving pressure and the geometry of confinement. Finally, we demonstrate controlled shaping of the nematic flow fronts by tuning the liquid crystal orientational profiles, which are capable of multi-stream velocity profiles and temperature responsive flow steering.



[1] J. G. Cuennet, A. E. Vasdekis, L. De Sio, D. Psaltis, Nature Photon. **5**, *234 (2011).*

[2] A. Sengupta, S. Herminghaus, C. Bahr, Appl. Phys. Lett. **101**, *164101 (2012).*

[3] A. Sengupta, U. Tkalec, M. Ravnik, J. M. Yeomans, C. Bahr, S. Herminghaus, Phys. Rev. Lett. **110**, *048303 (2013).*

[4] J. G. Cuennet, A. E. Vasdekis, D. Psaltis, Lab Chip **13**, *2721 (2013).*

[5] A. Sengupta, S. Herminghaus, C. Bahr, Liq. Cryst. Rev., *published online 17 Nov 2014, doi:10.1080/21680396.2014.963716.*

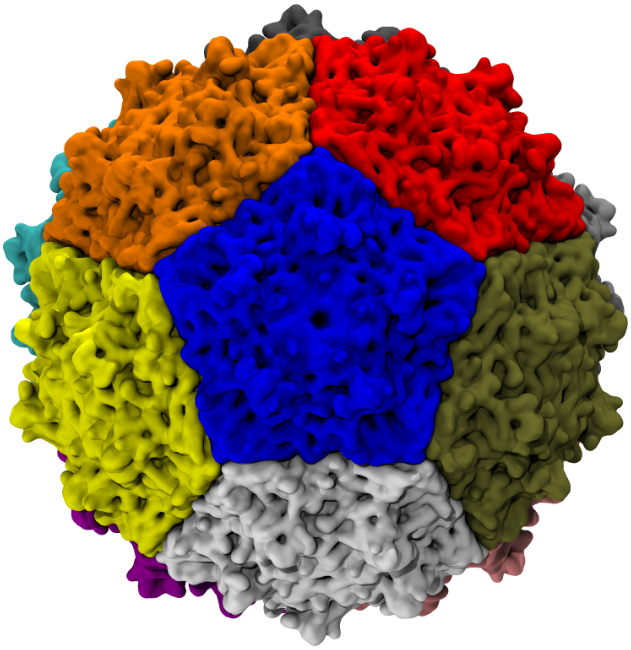
Quasi-rigid domains of proteins identified via dimensional reduction of distance fluctuation matrices

16:10
SM

L. Ponzoni[1*], G. Polles[1], V. Carnevale[2], C. Micheletti[1]

1 SISSA - Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, 34136 Trieste (Italy)
2 Institute for Computational Molecular Science, College of Science and Technology, Temple University. SERC, 1925 N. 12th Street, Philadelphia, PA 19122, USA
** lponzoni@sissa.it*

Large-scale movements in proteins often arise from the relative displacements of only few quasi-rigid domains. Developing computational strategies for identifying such domains from limited sets of alternative conformers can help unveil the functionally-oriented protein mechanics. One common obstacle towards this goal is the dependence of the domain identification on the clustering method used for partitioning amino acids in a given number of domains. A further challenge is the introduction of objective criteria for establishing the correct number of quasi-rigid domains. Here we present a novel domain-decomposition method, named SPECTRUS, which can overcome both obstacles. The method takes as input the matrix of amino acids pairwise distance fluctuations and uses the Laplacian spectral projection to optimally expose the innate clustering of the amino acids into quasi-rigid domains, thus making their identification practically independent of the chosen clustering scheme. In view of this robustness one obtains equivalent SPECTRUS subdivisions when using distance fluctuation matrices computed from thousands of conformers sampled by extensive MD simulations, or just a pair of alternative crystal structures, or even a single conformer used as a reference structure for an elastic network model. We further show that SPECTRUS can be profitably used to gain insight into the functional mechanics of molecules of very different size, from monomeric globular proteins to large macromolecular assemblies such as viral capsids.



17:10
C&T

Kinetics of adhesion and spreading of living cell at the charged interface

N. Ivošević DeNardis*, I. Ružić, J. Pečar Ilić, G. Pletikapić

Division for Marine and Environmental Research, Ruđer Bošković Institute, POB 180, 10000 Zagreb, Croatia
** ivosevic@irb.hr*

Adhesion and spreading of living algal cell and its corresponding ghost membrane in suspension at the charged interface is explored with comprehensive surface techniques (i.e. amperometry and atomic force microscopy) and mathematical modelling.

Kinetics of soft particle adhesion at the charged interface was not easy to access experimentally where completion of the whole process has been limited to the scale of the order of millisecond. The recorded amperometric signal of individual algal cell contains important information regarding dynamics of the corresponding process and reflecting collective surface properties of material itself. Reaction kinetics model enables determination of kinetics parameters from amperometric signal of the algal cell and reconstruction of individual states of adhesion process towards the final state formation[1].

Our results show the significant difference in kinetics of adhesion and spreading over the interface of intact algal cell and its ghost membrane. In the case of algal cell, the slower kinetics is associated with the release and spreading of intracellular material. The study of adhesion phenomena in single cell-electrode interaction is significant for relevant biological studies involving cell adhesion, cell fusion, cell activity and fundamental processes such as vesicular transport within and between cells.

[1] N. Ivošević DeNardis, I. Ružić, J. Pečar-Ilić, S. El Shawish, P. Ziherl (2012) Reaction kinetics and mechanical models of liposome adhesion at charged interface. Bioelectrochemistry *88:48–56.*

Surface tension-based mechanics of epithelia

17:30
C&T

M. Krajnc[1*], N. Štorgel[1,2], M. Rauzi[3], P. Mrak[4], J. Štrus[4], M. Leptin[3,5], P. Ziherl[1,2]

1 Jozef Stefan Institute, Ljubljana, Slovenia
2 Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia
3 European Molecular Biology Laboratory, 69117 Heidelberg, Germany
4 Biotechnical Faculty, University of Ljubljana, Ljubljana, Slovenia
5 Institute of Genetics, University of Cologne, D-50674 Cologne, Germany
** matej.krajnc@ijs.si*

We propose a mechanical model of epithelial tissues where cells are considered as incompressible units attached to the underlying elastic basement membrane. Cell shape changes are mediated through activities of various proteins, namely actins, cadherins, integrins, and myosin molecular motors. Cell energy is thus associated with the surface tension in actomyosin cortical network, with differential surface tension due to apico-basal polarity, and with negative surface tension due to cell-cell adhesion [1].

We establish a general model for simple, pseudostratified, double-layered, and stratified epithelia to study the conditions under which the particular morphology is stable. We apply this model to particular corrugated morphologies of simple epithelia found in various animal tissues such as the intestinal epithelium. We study the phase diagram of corrugated shapes and discover 5 qualitatively different epithelial classes: condensed, invaginated, evaginated, wavy, and flat. Apart from this we also study ventral furrow invagination in *Drosophila*. We argue that different cell populations in the developing embryo have distinct elastic properties which in our model arise from nonhomogeneous surface tension.

From the discrete model for homogeneous simple epithelial tissue we then develop an effective 2D continuum theory of epithelial cross section. The tissue is parametrized by the local curvature and carries an extra scalar function describing the local thickness, e.g. cell height. Apart from bending and stretching elasticity this model tissue is also characterized by the coupling between local curvature and local thickness. We derive the Euler-Lagrange equations and solve them for a particular boundary conditions.

[1] M. Krajnc, N. Štorgel, A. Hočevar. Brezavšček, P. Ziherl, A tension-based model of flat and corrugated simple epithelia, Soft Matter ***9****, 8368 (2013).*

17:50 C&T

Forces balance in the mitotic spindle

Nenad Pavin[1,*], Janko Kajtez[2], Anastasia Solomatina[2], Maja Novak[1], Matko Glunčić[1], Iva M. Tolić[2,3]

1 Faculty of Science, University of Zagreb, Zagreb, Croatia
2 Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany
3 Ruđer Bošković Institute, Zagreb, Croatia
** npavin@phy.hr*

During cell division, proper segregation of genetic material requires that sister chromatids of each chromosome attach to microtubule bundles known as k-fibers, extending from the opposite spindle poles via kinetochores, protein complexes on the chromosome. A key question is what forces act on k-fibers and kinetochores. According to the current paradigm, the forces on kinetochores are produced by k-fibers, bundles of microtubules extending between the spindle pole and the kinetochore. Here we show that a new class of microtubules, which we term bridging microtubules, interact with k-fibers thereby connect sister kinetochores and generate forces during metaphase and anaphase. We performed laser ablation of the outmost k-fiber. We found that after cutting, sister kinetochores, together with the intact k-fiber, the k-fiber stub extending from the kinetochore closer to the ablation site, and the microtubule between the k-fibers moved outwards, away from the central spindle. This result confirms that the bridging MTs are connected to k-fibers and the kinetochores into a single object. The existence of bridging microtubule implies that in the cutting experiment straightening of k-fibers should be faster in the case of a thicker bridging microtubule, which was indeed observed. Understanding the role of bridging microtubules in force generation and chromosome movements will shed light not only on the mechanism of chromosome segregation and the force balance in the entire spindle.

Cross-linking proteins facilitate formation of microtubule bundles

18:10
C&T

Marcel Prelogović[1], Lora Winters[2], Iva Tolić[2], Nenad Pavin[1]

1 Faculty of Science, University of Zagreb, Zagreb, Croatia
2 Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

During mitosis, microtubules (MTs) form a spindle which is responsible for proper segregation of chromosomes. In the fission yeast Schizosaccharomyces Pombe, the spindle is a bundle of MTs emanating from two spindle pole bodies and held together by cross-linking proteins . Our goal is to understand the dynamic properties of MTs interacting with cross-linking proteins and the role of cross-linking proteins in the formation of MT bundles. We introduce a theoretical model of MT bundling which describes angular movement of MTs around the spindle pole body driven by thermal forces and forces exerted by cross-linking proteins, described as elastic springs. If the number of cross-linking proteins connecting the MTs is above a critical number, attractive forces exerted by cross-linking proteins dominate over thermal forces at very small angles between MTs, causing MT-s to bundle. We identify stable bundles as the case where MTs are more likely to be bundled than not. Theory yields bundling probability as a function of length and cross-linking protein concentration and predicts parameters for which stable bundles form. In conclusion, these results provide an explanation for how the angular brownian motion and cross-linking proteins affect the formation of stable MT bundles.

9:00
N&B

Nanopores in SiN_x membranes

M. Lihter[1], S. Marion[1], A. Rađenović[2], T. Vuletić[1,*]

1 Institut za fiziku, Bijenička 46, 10000 Zagreb, Croatia
2 Laboratory of Nanoscale Biology, Institute of Bioengineering, School of Engineering, EPFL, 1015 Lausanne, Switzerland
** mlihter@ifs.hr*

Solid-state nanopores have become a new single-molecule tool in biophysics. In comparison to biological nanopores, they offer many advantages due to their robustness, high stability, tunable pore size and potential for integration into devices. A precursor in the preparation of a nanopore is a thin, solid supported membrane of e.g. SiN (thinner than 20 nm) or ultrathin 2D materials like graphene or MoS_2. Translocation of a macromolecule, e.g. DNA through a nm sized pore in such a thin membrane influences the ionic current of the surrounding electrolyte through the pore and electrical properties of the membrane itself. Both these transduction mechanisms provide single-molecule sensing capability and are being tested for an even finer role: DNA sequence readout - next generation DNA sequencing. Conventionally, nanopores are drilled in these membranes within a transmission electron microscope which is a tedious and resource intensive procedure. A latest development in this research field is a simple method of pore formation by the controlled dielectric breakdown of a membrane immersed in an electrolyte solution. We constructed a setup for nanopore characterisation and translocation measurements based on a commercial current preamplifier and some analog devices built in-house. It is also capable of performing the dielectric breakdown. We present the initial results on lambda DNA translocation events through a nanopore made in 20 nm SiN membrane by dielectric breakdown. Our goal is to establish the complete nanopore workflow in Zagreb: nanopore production, testing and its use as a novel tool in single-molecule studies.

2D Nanopores from Graphene to Molybdenum Disulfide

9:20
N&B

Ke Liu*, Jiandong Feng, Aleksandra Rađenović

Laboratory of Nanoscale Biology, Institute of Bioengineering, School of Engineering, EPFL, 1015 Lausanne, Switzerland
** ke.liu@epfl.ch*

New avenues of research in the field of single molecule experiment were opened with the advent of solid state nanopores. The major advantage of solid-state nanopores over their biological counterparts is that they can be easily integrated into devices compatible with other detection schemes[1, 2] such as a single molecule optical detection and manipulation. Recently, we made advances in using nanopore platform for its integration with 2D materials such as graphene or MoS_2[3]]. In this talk I will discuss comparative advantages of nanopores in two-dimensional nanosheets of layered transition metal dichalcogenides (TMDs).

[1] F. Traversi, C.Raillon, S. M. Benameur, K.Liu, S. Khlybov, M. Tosun, D. Krasnozhon, A.Kis and A.Radenovic, (2013) Detecting the translocation of DNA through a nanopore using graphene nanoribbons Nature Nanotechnology *8:939–945*

[2] A.Fanget, F. Traversi, S.Khlybov, P.Granjon, A.Magrez, L. Forró, and A. Radenovic, (2014) Nanopore Integrated Nanogaps for DNA Detection Nano Lett. *14(1):244–249*

[3] Liu, K., Feng, J., Kis, A. and Radenovic A., (2014) Atomically thin molybdenum disulfide nanopores with high sensitivity for DNA translocation ACS Nano *8:2504-2511*

9:40
N&B

Investigation of molecular ligand-receptor recognition tuned by cryoprotectants

I.Nikić[1,2*], I.Delač Marion[1], M.Leitner[2], A.Ebner [2],T.Vuletić[1]

1 Institut za Fziku, Bijenička 46, 10000 Zagreb, Croatia
2 Institute for Biophysics, Johannes Kepler University Linz, Gruberstraße 40, A-4020 Linz, Austria
** ivana.nikic7@gmail.com*

We studied (strept)avidin-biotin (SA/B) complex in the presence of cryoprotectants. Protein (receptor)-ligand pair SA/B is among the strongest non-covalent bonds in biology and has a broad range of applications [1]. There is a large amount of thermodynamic and structural data and the complex was researched under harsh conditions (e.g. extreme pH, organic solvents, and different temperature). Influence of commonly used cryoprotectants on this model system is of interest as it may convey information on preservation of protein functionality in cryo-storage. We investigated whether cryoprotectants interfere with the SA/B binding by single molecule force spectroscopy (SMFS) in liquid environment defined by the hydrogen-bond forming solvents (glycerol, ethylene glycol and DMSO) mixed with water (3-50 % cryoprotectant). Pure water and pure DMSO were also tested. We present the results obtained from the force-distance curves analysis and show the decrease in the binding affinity (the probability of the occurence of the specific binding) with the increase in the cryoprotectant fraction. The SA/B binding involves a number of polar and hydrogen bonds and water bridges [2]. The formation of the water bridges is less likely in the mixtures which might reduce the binding affinity. However, when the bond is formed, we do not find any specific dependence of the unbinding force on cryoprotectants. That is, for the used loading rate the measured force and extension of the molecules falls in the range reported in literature [3]. Solvophobic interaction in the studied solvent mixtures is commonly expected to be weaker than hydrophobic in water and thus SA/B binding may be expected to be weakened. However, a recent work indicates that glycerol does not diminish hydrogen-bonding ability of water, which is in agreement with our findings on the unbinding force [4].

[1] O. Livnah, E.A. Bayer, M. Wilchek, and J.L. Sussman (1993) Three-dimensional structures of avidin and the avidin-biotin complex Proc. Natl. Acad. Sci. *90:5076-5080.*

[2] H. Grübmuller, B. Heymann, and P. Tavan (1996) Ligand Binding: Molecular Mechanics Calculation of the Streptavidin-Biotin Rupture Force Science *271:997-999.*

[3] R. Merkel, P. Nassoy, A. Leung, K. Ritchie, and E. Evans (1999) Energy landscapes of receptor-ligand bonds explored with dynamic force spectroscopy. Nature *397:50-53.*

[4] J.J. Towey, A.K. Soper, and L. Dougan (2012) Molecular Insight Into the Hydrogen Bonding and Micro-Segregation of a Cryoprotectant Molecule J. Phys. Chem. B *116: 13898-13904.*

Role of the pH and electrolyte on the photocatalysis efficiency of the TiO_2 one dimensional nanomaterials

10:00
N&B

Atiđa Selmani[1*] Mario Špadina[1], Ida Delač Marion[2], Milivoj Plodinec[3], Marc G. Willinger[4], Harry D. Gafney[5] and Engelbert Redel[6]

1 Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, 10002 Zagreb, Croatia
2 Institute of Physics, Bijenicka 46, Zagreb, Croatia, Tel: +385 1 469 8887
3 Department of Material Physics, Rudjer Boskovic Institute, Bijenicka 54, 10000 Zagreb, Croatia
4 Department of Inorganic Chemistry, Fritz Haber –Institute of the Max Planck Society, Berlin, Germany
5 Department of Chemistry, City University of New York, Queens College, Flushing, New York 11367, United States
6 Karlsruhe Institute of Technology (KIT), Institute of Functional Interfaces (IFG), Germany
** aselmani@chem.pmf.hr*

Efficient photocatalysis of various pollutants in the environment is a complex process and include so many factors, i.e. morphological factors as well as acid-base properties of the metal oxide and has significant contribution to the overall photocatalysis efficiency. In spite of numerous studies dealing with effect of inorganic ions which are mosty focused on the heavy metals adsorption as well as ion exchange mechanism there is lack of the data in the literature with basic findings about effect of the surface pH and the ionic strength on the TiO_2 nanotubes and nanowires surfaces[1]. Detailed information about acid-base surface properties are essential, because pH is one of the most important factor that have effects on the photocatalysis performance and efficient purification of the organic contaminants due to surface charge dependence of the pH as well as interfacial electron transfer and surface/interface polarisation effects in regard to the ESAB model[2].

In this study we investigate the effect of the pH and ionic strength on the basic surface properties, i.e. surface charge and electrokinetic potential of the one dimensional TiO_2 nanomaterials. The comparative study of surface properties for the two TiO_2 nanomorphologies, nanotubes and nanowires show that the surface properties, i.e. pH_{iep} and pH_{pzc} of TiO_2 nanowires and nanotubes are independent of the electrolyte, but dependent on the morphology of the nanostructure. The observed results point to a the data point to a strong cation effect, i.e. higher cation affinity for the TiO_2 surface from electrokinetic measurements, potentiometric mass and electrolyte titrations. The isoelectric point shifts to higher pH, whereas the point of the zero charge shifts to the lower pH as the ionic strength increase. The findings emphasize the importance of the presence of common electrolyte, which can influence surface pH, and in turn, overall phoytocatalytic activity and efficiency. We believe the determination of surface charge as well as surface pH is quite important and crucial for a better understanding of TiO_2's photocatalytic properties.

[1] A. Piscopo, D. Robert, J. Weber, (2001) Appl. Catal., B Environ. ***35****, 117–124.*

[2] E. Look, H. D. Gafney, (2013) J. Phys. Chem. A. ***117****, 12268–12279.*

10:20 N&B

Lipid bilayer explosion driven by titan-oxide nanoparticles

M. Garvas[1,2], I. Urbančič[1], A. Testen[1,3,4], Z. Arsov[1,3], P. Umek[3,5], T. Koklič[1,3], J. Štrancar[1,3*]

1 Laboratory of Biophysics, Condensed Matter Physics Department, "Jožef Stefan" Institute, Jamova cesta 39, SI-1000 Ljubljana, Slovenia
2 Jožef Stefan International Postgraduate School, Jamova cesta 39, SI-1000 Ljubljana, Slovenia
3 Centre of Excellence NAMASTE, Jamova cesta 39, SI-1000 Ljubljana, Slovenia
4 Biotechnical Faculty, University of Ljubljana, Jamnikarjeva 101, SI-1000 Ljubljana, Slovenia
5 Laboratory of Magnetic Resonance and Dielectric Spectroscopy, Condensed Matter Physics Department, "Jožef Stefan" Institute, Jamova cesta 39, SI-1000 Ljubljana, Slovenia
** janez.strancar@ijs.si*

Outbreak of various nanomaterials is accompanied by human body exposure to the nanoparticles that can be uptaken and interact with the cells in a variety of potentially harmful ways. Cell plasma membrane disintegration is certainly one of them. In the present work we present the titan-oxide nanotube-induced cell membrane rupture that leads to unrestricted mitochondria relocation around the original cell location. To explain this, fluorescently-labeled model membrane vesicles are exposed to the fluorescently-labeled titan-oxide nanoparticles to identify the molecular contact between the membrane and nanoparticles via FRET and aggregation of nanoparticles during accumulation on the membranes revealed by homoFRET, both analyzed via flurescence microspectroscopy (FMS). Effect of charge on the particles and membranes will be presented. Finally the possible scenario of the membrane disintegration by nanoparticles will be discussed.

The behavior of the tension pore induced by a pore-forming agent

11:20
M2

B. Božič[1*], L. Kristanc[1], G. Gomišček[1,2]

1 Faculty of Medicine, University of Ljubljana, Vrazov trg 2, Ljubljana, Slovenia
2 Faculty of Health Sciences, University of Ljubljana, Zdravstvena pot 5, Ljubljana, Slovenia
** bojan.bozic@mf.uni-lj.si*

A typical behavior of giant phospholipid vesicles induced by the application of the pore forming agent nystatin was studied[1]. A theoretical model based on the osmotic phenomena that occur due to the size-discriminating pores was used[2]. The changes in tension-pore behavior observed in individual phospholipid vesicles, i.e., membrane bursts, slow vesicle ruptures and explosions, detected at increasing nystatin concentrations were explained. A significant shift of the typical vesicle behavior towards lower nystatin concentrations detected in the ergosterol-containing membranes and a slight shift towards higher nystatin concentrations detected in the cholesterol-containing membranes were interpreted. The role of the different mechanical characteristics of the membrane, i.e., the membrane's expansivity and the bending modulus, the line tension, and the lysis tension, in the tension-pore behavior was quantified. The sterol-induced changes could not be explained adequately on the basis of the mechanical characteristics, and were therefore interpreted mainly by considering the direct influences of the sterols on the membrane binding, the partition and the pore-formation process of nystatin.

[1] L. Kristanc, S. Svetina, G. Gomišček (2012) Effects of the pore-forming agent nystatin on giant phospholipid vesicles. Biochim. Biophys. Acta *1818:636–644.*

[2] L. Kristanc, B. Božič, G. Gomišček (2014) The role of sterols in the lipid vesicle response induced by the pore-forming agent nystatin. Biochim. Biophys. Acta *1838:2635–2645.*

11:40
M2

Fluctuation pressure of a membrane subject to hard wall constraints: a self-consistent approach

Bing-Sui Lu[1*], Rudolf Podgornik[1,2], A. C. Maggs[3]

1 Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, Jadranska ulica 19, SI-1000 Ljubljana, Slovenia
2 Department of Theoretical Physics, J. Stefan Institute, University of Ljubljana, Jadranska ulica 19, SI-1000 Ljubljana, Slovenia
3 Physico-chimie théorique–Gulliver, ESPCI-CNRS, 10 rue Vauquelin 75005 Paris, France
** bing-sui.lu@fmf.uni-lj.si*

I first present a quick introduction to fluid membranes, which are membranes that are resistant to changes in curvature but have no in-plane shear modulus. I describe a classic argument of Helfrich's that explains how the fluctuation pressure P that arises from confining a fluid membrane (of stiffness K) between two hard walls scales as the third power of the inverse distance between the walls. This argument relies on a postulated relation between the separation distance d and the mean square fluctuation σ^2 of the membrane, viz., $\sigma^2 = \rho\, d^2$, where ρ is temperature-*independent*. We propose a new approach via variational field theory that enables one to self-consistently derive the dependence of (i) P and (ii) σ^2 on (a) d and (b) temperature T. In this approach, we implement the hard wall constraints via a certain representation of the Heaviside function, which allows us to transform the constraints into energy terms in an effective Hamiltonian. We thus determine scaling relations for σ^2 and P for (i) an undulating membrane near a single hard wall, and (ii) a membrane between two hard walls. We find that $\sigma^2 \sim \sqrt{T/K}d^2$ and $P \sim d^{-3}$, and $P \to 0$ as $T \to 0$.

Charged Amphiphylic Ligands of Nanoparticles Increase Lateral Compaction of Membranes. Nanomechanical and Thermotropic Study of Model Lipid Membranes in High Ionic Strength Solutions

12:00
M2

S. Šegota[1,*], D. Vojta[2], D. Kendziora[3], I. Ahmed[3], Lj. Fruk[3], G. Baranović[2]

1 Division for Marine and Environmental Research, Ruđer Bošković Institute, POB 180, Zagreb, Croatia
2 Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, POB 180, Zagreb, Croatia
3 DFG - Center for Functional Nanostructures, Karlsruhe Institute for Technology,76131 Karlsruhe, Germany
** ssegota@irb.hr*

The research of the nanoparticle (NP) delivery systems and the use of NPs both for diagnostic and therapeutic purposes have created a need for understanding the complex interactions of NPs with cells. Membrane-NP interactions are of crucial importance both for the cell uptake and toxicological investigations. For that reason, lipids that are the cell membrane building blocks, have been used as simplified model systems to study not only the mechanical properties of the membranes and their interactions with different molecular species, but also their structural organization in, for example, marine ecosystems, which are particularly sensitive to the toxicological environmental effects[1].

The presence of hydrophobic NPs embedded within a lipid bilayer, can lead to rearrangement of lipid nolecules by modifying interactions amongst the lipd headgroups and/or acyl tails. Therefore, research towards the examination of interaction of NP within lipid membranes using transmission infrared spectroscopy and force spectroscopy (FS) have been undertaken.

Our research deciphered interactions of hydrophobic NP with model membranes through their delicate response in physiological and seawater environment. Functionality of the NP has been related to the organisation and fluidity of the model lipid membrane. The formation of lipid/NP assemblies containing hydrophobically modified NPs showed specific effects on the later compaction of the supported lipid bilayers arround NPs in both media.

*[1] S. Šegota *, D. Vojta, G. Pletikapić, G. Baranović, (2014)* Chem. Phys. Lipids*, in Press*

12:20
M2

Pearling instability of membrane tubes driven by curved proteins and actin polymerisation

U. Jelerčič[1*], N. S. Gov[2]

1 Jožef Stefan Institute, Department of Theoretical Physics, Jamova 39, SI-1000 Ljubljana, Slovenia
2 Department of Chemical Physics, The Weizmann Institute of Science, P.O. Box 26, Rehovot, Israel 76100
** urska.jelercic@ijs.si*

Membrane deformation inside living cells is crucial for the proper shaping of various intracellular organelles and is necessary during the fission/fusion processes that allow membrane recycling and transport (e.g. endocytosis). Proteins that induce membrane curvature play a key role in such processes, mostly by adsorbing to the membrane and forming a scaffold that deforms the membrane according to the curvature of the proteins. In this paper we explore the possibility of membrane tube destabilisation through a pearling mechanism enabled by the combined effects of the adsorbed curved proteins and the actin polymerisation they may recruit. The pearling instability can furthermore serve as the initiation for fission of the tube into vesicles. We find that adsorbed proteins are more likely to stabilise the tubes, while the actin polymerisation can provide the additional constrictive force needed for the robust instability. We discuss the relevance of the theoretical results to in-vivo and in-vitro experiments.

Open collaboration that uses nmr data to judge the correctness of phospholipid glycerol and head group structures in molecular dynamics simulations

12:40
M2

M. S. Miettinen[1*], NMRlipids collaborators[2]

1 Department of Physics, Freie Universität Berlin, Germany
2 nmrlipids.blogspot.fi
** markus.miettinen@iki.fi*

We compare the C-H order parameters measured by Nuclear Magnetic Resonance (NMR) experiments to those predicted by 13 different molecular dynamics (MD) simulation models. We focus on the order parameters of the lipid headgroups and glycerol backbones in phospholipid bilayers.

Only two of the models (CHARMM36 [1] and Maciejewski–Rog [2]) give a reasonable agreement with experiments for a fully hydrated lipid bilayer.

We then compare (for the two best-performing models at full hydration and for the Berger model [3], the most used lipid model in the literature) to NMR experiments the changes in the order parameters as a function of hydration level, NaCl and $CaCl_2$ concentrations, and cholesterol content. The results clearly show that the glycerol and headgroup structures in the Berger model are not realistic, the Na^+ ion partitioning is significantly too strong and cholesterol-induced structural changes are overestimated. The CHARMM36 and Maciejewski–Rog perform better, but the Na^+ partitioning is too strong at least in the latter.

This is an open science project that is progressed at `nmrlipids.blogspot.fi`. All the results and discussions are available at that address.

[1] J. B. Klauda, . . . , R. W. Pastor. (2010) J. Phys. Chem. B *114:7830.*

[2] A. Maciejewski, . . . , T. Rog. (2014) J. Phys. Chem. B *118:4571.*

[3] O. Berger, O. Edholm, F. Jähnig. (1997) Biophys. J. *72:2002.*

List of participants

Michal Belička	Karl-Franzens-Universität Graz	michal.belicka@uni-graz.at
Bojan Božič	Faculty of Medicine, University of Ljubljana	bojan.bozic@mf.uni-lj.si
Ida Delač Marion	Institute of Physics, Zagreb	idelac@ifs.hr
Barbara Geier	University of Graz, Institute of Molecular Biosciences	barbara.geier@uni-graz.at
Danijel Grgičin	Institute of Physics, Zagreb	dgrgicin@ifs.hr
Peter Heftberger	University of Graz, Institute of Molecular Biosciences	peter.heftberger@uni-graz.at
Nadica Ivošević DeNardis	Ruđer Bošković Institute, Zagreb	ivosevic@irb.hr
Urška Jelerčič	Jozef Stefan Institute, Ljubljana	urska.jelercic@ijs.si
Ivan Jurić	Institute of Physics, Zagreb	ijuric@ifs.hr
Benjamin Kollmitzer	University of Graz, Institute of Molecular Biosciences	Benjamin.kollmitzer@uni-graz.at
Matej Krajnc	Jozef Stefan Institute, Ljubljana	matej.krajnc@ijs.si
Martina Lihter	Institute of Physics, Zagreb	mlihter@ifs.hr
Ke Liu	École Polytechnique Fédérale de Lausanne, Switzerland	ke.liu@epfl.ch
Bing-Sui Lu	University of Ljubljana, Faculty of Mathematics and Physics	bing-sui.lu@fmf.uni-lj.si
Sanjin Marion	Institute of Physics, Zagreb	smarion@ifs.hr
Cristian Micheletti	SISSA, Trieste	michelet@sissa.it
Markus Miettinen	Department of Physics, Freie Universität Berlin	markus.miettinen@iki.fi
Ivana Nikić	Institute of Physics, Zagreb	ivananikic7@gmail.com
Georg Pabst	University of Graz, Institute of Molecular Biosciences	georg.pabst@uni-graz.at
Nenad Pavin	Faculty of Science, University of Zagreb	npavin@phy.hr
Guido Polles	SISSA, Trieste	gpolles@sissa.it
Luca Ponzoni	SISSA, Trieste	lponzoni@sissa.it
Santosh Prasad Gupta	University of Graz, Institute of Molecular Biosciences	santosh.gupta@uni-graz.at
Marcel Prelogović	Faculty of Science, University of Zagreb	mprelogovic@phy.hr
Suzana Šegota	Ruđer Bošković Institute, Zagreb	ssegota@irb.hr
Atiđa Selmani	Department of Chemistry, Faculty of Science, University of Zagreb	aselmani@chem.pmf.hr
Antonio Šiber	Institute of Physics, Zagreb	asiber@ifs.hr
Janez Štrancar	Jožef Stefan Institute and Centre of Excellence NAMASTE, Ljubljana	janez.strancar@ijs.si
Antonio Suma	SISSA, Trieste	antonio.suma@sissa.it
Uroš Tkalec	Institute of Biophysics, Faculty of Medicine, University of Ljubljana	uros.tkalec@ijs.si
Iztok Urbančič	Jožef Stefan Institute, Ljubljana	iztok.urbancic@ijs.si
Tomislav Vuletić	Institute of Physics, Zagreb	tvuletic@ifs.hr
Primož Ziherl	Faculty of Mathematics and Physics, University of Ljubljana, and Jozef Stefan Institute, Ljubljana	primoz.ziherl@ijs.si