

BOOK OF ABSTRACTS

XVIII CHRISTMAS BIOPHYSICS WORKSHOP

Hotel Nevada, Tarvisio, Italy

16-17 December 2024

Schedule

Monday 16/12/2024

Session I. Membranes, vesicles, and cells – Chair: C. Micheletti

- 10:30 - 10:50 Pabst
- 10:50 - 11:10 Haidinger
- 11:10 - 11:30 Andresek
- 11:30 - 11:50 Popović
- 11:50 - 12:10 Železnik

Session II. Biopolymers and Biological Systems I – Chair: A. Šiber
15:00 - 15:20 Zechner

- 15:20 - 15:40 Idiyatullina
- 15:40 - 16:00 Bukina
- 16:00 - 16:20 Di Marco
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Session III. Nanomaterials - Chair: G. Pabst

- 17:10 - 17:30 Delač
 - 17:30 - 17:
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Tuesday 17/12/2024

Session IV. Biopolymers and Biological Systems II – Chair: T. Vuletić

- 9:30 - 9:50 Svetina
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ABSTRACTS

Monday 16/12/2024 10:30 - 10:50

Metal ion cofactors modulate integral enzyme activity by varying differential membrane curvature stress

Georg Pabst
University of Graz

Metal ions are well-known cofactors of protein function and stability. In the case of the integral membrane enzyme OmpLA (outer membrane phospholipase A) the active dimer is stabilized by calcium ions. We studied the lipid hydrolysis kinetics of OmpLA in charge-neutral and charged membranes with symmetric or asymmetric transbilayer lipid distributions. In charge-neutral membranes, OmpLA was more active in symmetric bilayers due to the lower differential curvature stress between membrane leaflets. Strikingly, this behavior was completely reversed in charged bilayers. Measurements revealed intrinsic molecular shape changes in the charged lipids upon addition of calcium. This effectively reduces the differential curvature stress in charged asymmetric membranes leading to increased protein activity. This conclusion is further supported by similar effects observed upon the addition of sodium ions, which also alter the shape of the lipids, but do not specifically interact with the protein. Additional lipid-protein interactions likely contribute to this phenomenon. Our findings demonstrate that ion cofactors not only interact directly with membrane proteins but also modulate protein activity indirectly by altering the effective molecular shape of charged lipid species.

Monday 16/12/2024 10:50 - 11:10

Bending strongly curved lipid membranes: inverted hexagonal phases under osmotic stress

Angelika Haidinger
Graz University Technology, Institute of Theoretical and Computational Physics

The morphology of lipid membranes is governed by the balance between external stress and the intrinsic curvature of individual lipids. We combine molecular dynamics simulations and SAXS measurements to investigate inverted hexagonal phases under osmotic stress. Samples were prepared using Rapid Solvent Exchange (RSE) with a consistent lipid-tricosene composition of 12 wt% tricosene, and osmotic stress was induced by polyethylene glycol (PEG 8000). A key focus of our analysis is the bending rigidity, providing insights into the mechanical properties of the lipid membranes and the influence of osmotic stress on membrane curvature. The bending rigidity extracted from the experiments matches literature values, decreasing with increasing temperature.

Monday 16/12/2024 11:10 - 11:30

Elasticity of supported epithelia based on interfacial surface tensions

Urska Andresek
Jozef Stefan Institute

During the course of life of animal organisms, epithelial tissues undergo extensive deformations--first to form organs during embryogenesis and later to preserve organ's integrity and function in adulthood. To what extent these deformations resemble that of non-living elastic materials and in what ways they differ due to specific microscopic cell mechanics is not well understood. We derive an elasticity theory of epithelia, supported by the basement membrane and the stroma, in which the mechanics of individual cells are dominated by differential interfacial surface tensions. We start at a single-cell level, and describe tissue in cross section as a chain of droplet-like cells, subjected to surface tensions due to cell-cortex contractions and cell-cell adhesion. Upon performing a continuum limit, we obtain a harmonic elasticity theory that describes how intracellular forces and the interaction with supporting structures interplay in determining critical conditions for the elastic instability, where flat tissue loses stability and either buckles out of plane or forms periodic wrinkling patterns. Unlike in ordinary elastic layers, where stresses are distributed along the whole thickness of the layer, our model assumes cell-surface stresses while considering cells' interiors liquid-like. Due to this distinct origin of elasticity, the scaling of key physical quantities, including the critical load to induce elastic instability and the wavelength of the wrinkling pattern, with layer's thickness is fundamentally different than in ordinary elastic (bi)layers. Our theory also naturally describes reversal of the groove-to-crest thickness-modulation phase--a known shape feature, observed in epithelia, that cannot be explained by the elasticity theory of standard elastic bilayers. In all, our work provides a guideline for understanding how cell surface tensions and the interaction of tissues with supporting structures collectively shape epithelia during morphogenesis. Specifically, it provides a set of testable analytical results that characterize the contribution of surface mechanics to the elastic properties and shapes of epithelial monolayers.

Monday 16/12/2024 11:30 - 11:50

Disorder and order of cell packing in developing fruit fly wing epithelium

Marko Popović
Max Planck Institute for Physics of Complex Systems, Dresden

Tightly packed epithelial layers of cells are one of the main types of biological tissues. During tissue development, cellular packings commonly remain disordered, with a broad distribution of cell sizes. This pattern is also evident during the development of the wing of the fruit fly *D. melanogaster*. We analyze the dynamics of individual cells in developing fruit fly wing over 13 hours of development and find that a simple model of the cell cycle can explain the observed cell size distribution with no fitting parameters. Furthermore, we find that most of the polydispersity of cell sizes can be accounted for by the cell cycle. Strikingly, at a later stage of development, as cell proliferation halts, cellular packing transitions to an ordered hexagonal packing. We propose that this transition is controlled by the reduction of cell size polydispersity. To test this hypothesis we study how the cell size polydispersity controls order

of cell packing in the vertex model of epithelial tissues, and we compare our results with experimental observations.

Monday 16/12/2024 11:50 - 12:10

Mechanics of cell aggregates as models of tumors and tumor spheroids

Urban Železnik
Jožef Stefan Institute

The vertex model (VM) is a reliable tool for modeling two-dimensional biological epithelial tissues, but certain limitations emerge in three-dimensional systems due to the computational complexity of the problems. This complexity arises mainly from the intricate topological changes occurring in active tissues. The Graph Vertex Model (GVM) allows us to model three-dimensional epithelial tissues, such as tumors and tumor spheroids, where epithelial cells are represented as polyhedra. The model offers a simpler implementation of topological transformations within the tissue, including cellular rearrangements (T1 topological transitions in two-dimensional representation) and cell divisions. Additionally, the GVM generalizes topological transformations in both two and three dimensions. Here, we represent tumors with free boundary conditions that grow due to cell divisions on the outer layer of the tumor. The shapes of growing tumors depend on the fluctuations at cell edges, the frequency of cell divisions, and the mechanical tension between the necrotic core of the tumor and the outer layer of dividing cells.

Monday 16/12/2024 15:00 - 15:20

Stochastic processes in cells and tissues

Christoph Zechner
SISSA, Trieste, Italy

Monday 16/12/2024 15:20 - 15:40

Differences in Proteome Composition Among Pelagibacterales (Marine Bacteria) Living Under Different Salinity Regimes

Aisha Idiyatullina
University of Ljubljana

Habitat significantly influences its inhabitants, and adaptation to the environment is a lengthy and complex process. It is not yet clear how environmental properties impact protein structure. Some studies have examined cytoplasmic microbial proteins in hypersaline conditions, revealing a shift in amino acid composition toward acidity. However, similar studies for

membrane proteins, particularly rhodopsins, are lacking. Previously, we analyzed metagenomic data from marine, brackish, and freshwater environments and found correlations: major differences in amino acid composition accumulated in the outer part, with more polar amino acids in freshwater and more negative ones in marine environments. In this study, we aimed to refine our results by eliminating the influence of different taxonomies and protein functions. Thus, we focused solely on Pelagibacterales and Acidimicrobiales rhodopsins to explore correlations in amino acid composition differences across various habitats.

Monday 16/12/2024 15:40 - 16:00

Structural motif stability of bacteriophage MS2 RNA packaging signals upon changes in their flanking sequence

Veronika Bukina
Jožef Stefan Institute

The RNA motifs can be responsible for specific important functions. For instance, in bacteriophage MS2, they serve as packaging signals (PSs), which play a crucial role in binding viral coat proteins during capsid assembly. This work aims to analyse motif structural stability on the example of the well-studied MS2 virus. As a consequence of current experimental studies, which reveal the multiple putative PS sites across the MS2 RNA genome, we focus on 14 RNA motifs of the virus, including the most widely known TR hairpin. The study of motif stability involves manipulating the flanking sequences surrounding them and comparing various measures calculated from their secondary structure, such as structure probability, ensemble defect, and Shannon entropy. To verify the tertiary structures of these RNA segments, the oxDNA software is employed. Our results show the stability of certain motifs regardless of the presence or absence of sequences around them, even when the nucleotide content of flanking sequences is randomized. Conversely, other unstable motifs are stabilized by genome or flanking sequences that tell us about the importance of the particular structure as well as of the genome sequence. The outcome of this work is beyond viral PS structural stability, extending to applications in RNA binding protein (RBP) studies and more.

Monday 16/12/2024 16:00 - 16:20

All-atom simulations elucidate the molecular mechanism underlying RNA-membrane interactions

Salvatore Di Marco
SISSA, Trieste, Italy

RNA-membrane interactions are starting to emerge as an important organizing force in both natural and synthetic biological systems. Recently, RNA molecules were discovered to be present on the extracellular surface of living cells, where they mediate intercellular signalling. Furthermore, RNA-membrane interactions influence the efficacy of lipid-based RNA delivery systems. However, the molecular terms driving RNA localization at the membrane remain poorly understood. In this work, we investigate how RNA-phospholipid membrane interactions

occur by means of all atom simulations. We find that among the four RNA nucleobases, guanine exhibits the strongest interaction with the membrane due to extensive hydrogen-bond formation. Additionally, we show that intra-RNA base-pairing present in organized RNA structures significantly hinders RNA binding to the membrane. Elucidating the molecular details of RNA-membrane association will importantly contribute to improving the design of RNA-based drugs as well as lipid-based RNA delivery systems and to parsing out RNA transport and localization mechanisms.

Monday 16/12/2024 16:20 - 16:40

Hunting metal ions in RNA structures using molecular simulations

Giovanni Bussi
SISSA, Trieste, Italy

Monday 16/12/2024 17:10 - 17:30

Stability of organic molecule modifications of CVD-synthesized monolayer MoS₂

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Focus of our research is the modification of the two-dimensional (2D) materials' properties by utilizing a layer of organic molecules. Starting point of work presented here was the synthesis of the 2D material - monolayer MoS₂ using chemical vapor deposition (CVD), followed by transfer and characterization. Next step was studying effects of prolonged exposure to ambient conditions and different solvents, in order to develop optimal procedures and to distinguish the effects of the solvent from those of the organic molecules. During our research, we developed a simple method for modification of 2D materials by deposition of the organic molecule solution on the 2D material [1]. We further investigated the stability of our samples modified with L63MS (6-(4,5-dihydro-1H-imidazol-3-ium-2-yl)2(naphthalene-2-yl)benzothiazole methanesulfonate) molecule, as well as the reversibility of this modification. By analyzing the optical signatures of the samples using photoluminescence spectroscopy (PL), Raman spectroscopy, and surface quality using atomic force microscopy (AFM), we demonstrated that the modification of 2D MoS₂ with L63MS molecule leads to a stable surface modification that retains its optical signature, while heating of the modified samples restores their original optical signatures, indicating the re-establishment of the optical properties of the pristine MoS₂ [2]. Lastly, we were interested in the evolution of optical properties of MoS₂ monolayers modified with organic molecules during thermal treatment. During these experiments, the interaction of the MoS₂ and L63MS system with laser light at varying temperature regimes

revealed unexpected changes in the material's physical and electronic properties, namely, formation of organic molecule agglomerates on 2D material. This discovery led us to conduct a series of targeted experiments aimed at deciphering the effects of laser parameters, such as wavelength, intensity, and exposure duration on the 2D MoS₂ modified with L63MS during thermal treatment.

[1] A.L. Brkić et al., *Nanomaterials* 13, 2115 (2023)

[2] A.L. Brkić et al., *Nanotechnology* 36, 065702 (2025)

Monday 16/12/2024 17:30 - 17:50

Collagen I-binding dynamics with and without hyaluronic acid-coated gold nanoparticles:
Implications for enhanced wound healing applications

Atida Selmani¹, Ramona Jeitler, Christina Glader, Ivan Vidaković, Nataša Vujičić, Martin Sterrer, Nives Matijaković Mlinarić, Karin Kornmüller and Eva Roblegg

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Gold nanoparticles (AuNPs) are used in wound healing therapy. They can penetrate the stratum corneum, trigger the expression of fibroblasts and growth factors and thus promote collagen formation, neovascularization and the formation of granulation tissue.¹ At the wound site, they interact with components of the extracellular matrix (ECM), which is a complex and dynamic highly organized network of macromolecules such as collagens (I and III) and hyaluronic acid (HA) as well as proteoglycans and glycosaminoglycans.² These interactions result in the formation of a protein corona affecting the primary identity of AuNPs. Thereby, the conformation of the proteins on the surface depends on the physical and chemical environment and is a dynamic process that determines the functionality and stability of the AuNPs.

This study aimed at building a sound understanding of interaction dynamics between uncoated (AuNPs) and HA coated AuNPs (AuNPs-HA) taking into account particle size. First, 17 nm and 55 nm AuNPs with and without HA were prepared according to protocols of Selmani et al.³ Each particle type was analyzed by X-ray photoelectron spectroscopy (XPS), Raman and photoluminescence (PL) spectroscopy and Fourier-transform infrared spectroscopy (FTIR). The morphology was visualized with atomic force microscopy (AFM), while size and surface charge were examined by dynamic (DLS) and electrophoretic light scattering (ELS). The optical properties of AuNPs, i.e., surface plasmon resonance (SPR) were determined with UV-VIS spectrophotometry. Second, AuNPs were incubated in collagen I buffer dispersions at relevant concentrations, considering physiological/treatment conditions, in particular pH 4 (lactate buffer) and 7.4 (PBS buffer) at 10 mM buffer concentrations. The interactions between AuNPs and collagen I were studied with DLS, ELS, FTIR, UV-Vis spectrophotometry, fluorescence quenching titration, circular dichroism and SDS-PAGE.

The spectral differences between HA-AuNPs and AuNPs were confirmed by XPS, Raman, PL and FTIR. The sizes of AuNPs-HA (16 nm and 54 nm) were similar to those of AuNPs (17 and 57 nm). The zeta potential for the smaller AuNPs was -23 mV, that of the 57 nm particles -33 mV. In comparison, the 16 nm and 54 nm AuNPs-HA had a zeta potential of -30 mV and -40 mV, respectively, indicating that they are colloiddally stable. The SPR peak of the AuNPs-HA displayed a shift toward smaller wavelengths (i.e., blue shift). After dispersion in collagen I,

adsorption on the particle surface was confirmed by FTIR independent of size and HA functionalization. This correlated with an increase in particle size and changes in zeta potential. As expected, the zeta potential decreased for AuNPs-HA and changed to positive for AuNPs. The SPR peaks of both AuNP types shifted to higher wavelengths (i.e., red shift). In addition, at pH 4, changes in the secondary structure of collagen I were observed for all NP types except 17 nm AuNPs. At pH 7.4, both AuNPs and AuNPs-HA showed changes in the secondary structure of collagen I.

The results provide first insights into interaction dynamics between AuNPs or AuNPs-HA and collagen I as the dominant component of the ECM. It is evident that, in addition to surface functionalization, physiological conditions such as pH value also exert a significant influence on the rational development of formulations for wound treatment.

1. Mendes et al., ACS Biomater. Sci. Eng. 2020; 6:5132.

2. Karamanos, N.K.; Tzanakakis G.N. Curr. Opin. Pharmacol. 2012; 12:220.

3. Selmani et al., Nanomaterials 2023; 13:1878.

Monday 16/12/2024 17:50 - 18:10

Composites of calcium carbonate and zinc oxide nanoparticles for the development of antibacterial and biocompatible implants

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Loss of implant function is a common complication in orthopedic and dental surgery, often resulting in significant trauma. With the ageing population and increasing life expectancy, the number of revision procedures due to peri-implant infections is projected to rise by 42–149% by 2040 [1]. Among the primary causes of implant failure are peri-implant infections, which are frequently associated with polymicrobial biofilm formation on titanium surfaces. These biofilms are a major risk factor for inflammatory processes in the surrounding tissues, ultimately leading to implant failure and consequently resulting in implant removal. Metal-based nanoparticles (NPs) have emerged as promising antimicrobial agents due to their efficacy at low concentrations [2,3]. Zinc oxide nanoparticles (ZnO NPs) are particularly attractive due to their biocompatibility with human cells and low cytotoxicity at low concentrations.

In this study, ZnO NPs of various sizes and morphologies were incorporated into a composite coating with epitaxially grown calcium carbonate (CaCO₃) on titanium surfaces. To enhance CaCO₃ resorption, vaterite—the most unstable and soluble polymorph of CaCO₃—was utilised, given its better suitability for restorative applications. The coated samples were characterised using Fourier-transform infrared spectroscopy (FTIR) and X-ray diffraction analysis (XRD), with morphology assessed by scanning electron microscopy (SEM) and surface properties evaluated via water contact angle measurements. Zinc ion release was quantified using inductively coupled plasma mass spectrometry (ICP-MS). The antimicrobial

efficacy of the coatings was tested against *Staphylococcus aureus* (*S. aureus*), *Staphylococcus epidermidis* (*S. epidermidis*), and *Candida albicans* (*C. albicans*).

Results demonstrated successful epitaxial growth of vaterite on titanium surfaces. The Zn ions released from ZnO NPs significantly influenced the morphology of vaterite. ICP-MS analysis confirmed that the concentration of released Zn ions remained below 2 µg/mL. The treated titanium surfaces exhibited robust antimicrobial activity, achieving over 90% reduction in microbial viability for *S. aureus*, *S. epidermidis*, and *C. albicans*. Comparable antimicrobial efficacy was observed for sphere-like and rod-like ZnO NPs. This research contributes to the development of an innovative CaCO₃-ZnO NP composite for producing antibacterial and biocompatible titanium implants, a novel approach that has not been previously explored.

[1] I. Shichman, et al, *Arthroplast Today* 2023, 21, 101152.

[2] Y. Li, W. Xiong, et al. *J Biomed Mater Res A* 2014, 102, 3939.

[3] A. Turlybekuly, et al., *Materials Science and Engineering C* 2019, 104.

[4] A. Lucas, et al., *International Journal of Inorganic Materials* 2001, 3, 87.

Monday 16/12/2024 18:10 - 18:30

THE ROLE OF ADSORPTION IN STABILIZATION OF TiO₂ NANOPARTICLES WITH DIFFERENT CLASSES OF DISPERSANTS

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The application of nanotechnology in the development of new materials for different applications has enabled exceptional progress in various areas of human activity. Among the nanomaterials, TiO₂ nanomaterials (TiNM) are the second most often used ones in commercially available products, due to their exceptional properties.¹ In a large number of applications, TiNM are used in the form of suspensions. Considering that the effectiveness,² but also the toxicity of nanomaterials, and thus their impact on human health and the environment, depend on the degree of aggregation of their particles, determining the conditions under which nanomaterial suspensions are stable is extremely important for their safe application.³ Nanoparticles of sizes smaller than 100 nm have a pronounced tendency to aggregate in order to reduce the surface to volume ratio and thus the surface energy of the system. Therefore, in order to obtain stable suspensions, it is necessary to modify the surface of nanomaterials, either by adsorption of dispersants or by chemical modification of the surface.⁴ Despite numerous investigations of TiNM stabilities, the choice of efficient dispersant is still based on trial and error.

Motivated by this we have investigated interactions of four different dispersants with TiNP in order to determine the relationship between adsorption properties and the stability of TiNP suspensions in water. Structurally different polyelectrolytes (polyacrylic acid (PAA) and polyvinylpyrrolidone (PVP)) and surface-active substances (sodium dodecylbenzenesulfonate (SDBS) and Triton X-100 (TX-100)) were chosen as representatives of the most commonly used dispersants in various technological applications.² TiNP suspensions were prepared via ultrasonication using three different concentrations of each dispersant. Stability of such prepared suspensions was monitored during one month, using electrokinetic and dynamic light

scattering measurements. Obtained results confirmed 30-day stability of TiNP suspensions stabilized with lower concentrations of PAA and SDBS and the highest investigated PVP concentration, while showing that TX-100 was not good for stabilization of TiNP suspensions. Additionally, point of zero charge for TiNP-dispersant complexes was determined where applicable. Adsorption isotherms and adsorption kinetics were determined spectrophotometrically for each dispersant. It was found that adsorption of all dispersants follows the pseudo-second order kinetics. Also, the amount of adsorbed dispersant was lowest for TX 100, which could correlate with lowest suspension stability. The obtained results represent potential bases for developing rational approach in the preparation of stable TiNM dispersions.

Acknowledgments. This work was financially supported by the European Union's Horizon-RIA project, Surface Transfer of Pathogens (STOP), Grant agreement ID: 101057961.

- (1) Sahare, P. *et al.* Engineered Titania Nanomaterials in Advanced Clinical Applications. *Beilstein J. Nanotechnol.* **2022**, *13*, 201–218.
- (2) Farrokhpay, S. A Review of Polymeric Dispersant Stabilization of Titania Pigment. *Advances in Colloid and Interface Science* **2009**, *151* (1–2), 24–32.
- (3) Andreani, T. *et al.* The Critical Role of the Dispersant Agents in the Preparation and Ecotoxicity of Nanomaterial Suspensions. *Environ. Sci. Pollut. Res* **2020**, *27* (16), 19845–19857.
- (4) Faure, B. *et al.* Dispersion and Surface Functionalization of Oxide Nanoparticles for Transparent Photocatalytic and UV-Protecting Coatings and Sunscreens. *Science and Technology of Advanced Materials* **2013**, *14* (2), 023001.

Tuesday 17/12/2024, 9:30 – 9:50

On revealing Piezo1 conformational states

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Piezo1 is a mechanosensitive protein known to respond to mechanical forces acting on cellular membranes. The cryo-EM studies of Piezo1 molecule solubilized by detergents have shown that it is a homotrimer with a look of a propeller whose central part containing the pore is formed by transmembrane helices of all three subunits, and each of its three blades belongs to only one subunit. Typical action that causes the opening of normally closed pore is an increase of membrane lateral tension. Piezo1 conformations with an open pore are not stable which is evidenced by that the channel, at still tensed membrane, makes a transition into the so called deactivated state. This system's property suggests that the number of Piezo1 conformational states could be multiple. Here we show that it is possible to get some information about the multiplicity of Piezo1 conformational states from the analysis of cryo-EM measurements of shapes of phospholipid vesicles containing a single Piezo1 molecule. By assuming that each of the blades may attain two conformations independently on the conformational states of the other two blades, and introducing a model of blade elastic properties we examined shapes of seven such vesicles measured by Haselwandter et al. (Proc.

Nat. Acad. Sci, 119, e2208027119, 2022). Their shape behavior could be resolved on the basis of three different Piezo1 conformations.

Tuesday 17/12/2024, 9:50 - 10:10

Normalized topological indices discriminate between architectures of branched macromolecules

Domen Vaupotič
Jožef Stefan Institute

Branching architecture characterizes numerous systems, ranging from synthetic (hyper)branched polymers and biomolecules such as lignin, amylopectin, and nucleic acids to tracheal and neuronal networks. Branched macromolecules exhibit unique properties, such as compactness and high surface functionality, which influence their physical behaviour. These properties are often studied by mapping macromolecules to mathematical trees and characterized by topological indices. However, comparing molecules of different sizes is challenging due to the strong dependence of topological indices on the number of nodes in a tree. We propose a new method for normalizing topological indices based on the estimates of their probability density functions. Using two indices, we create a phase space that clearly distinguishes between various branching architectures. This approach is demonstrated on RNA and different coarse-graining methods and has broad applications in fields like polymer physics, green chemistry, and bioengineering.

Tuesday 17/12/2024, 10:10 - 10:30

Cation-dependent aggregation of polyglutamine beta sheets

Douwe Jan Bonthuis
TU Graz

The presence of expanded poly-glutamine (polyQ) repeats in proteins is directly linked to the pathogenesis of several neurodegenerative diseases, such as Huntington's, Alzheimer's and Parkinson's diseases. These diseases are characterized by the aggregation of misfolded proteins, such as amyloid fibrils, which are toxic to cells. However, the molecular and structural basis underlying the aggregation of proteins containing expanded polyQ repeats remain poorly understood. We use atomistic molecular dynamics to simulate an antiparallel polyQ beta sheet in water and determine the free energy of different cations as a function of distance from the polyQ surface. Incorporating the simulated free energy profiles into continuum theory, we show that the disjoining pressure between beta sheets exhibits pronounced negative regions, indicating a cation-dependent aggregation tendency.

Tuesday 17/12/2024, 10:30 - 10:50

Phase behavior of polymer/solvent mixtures: field-theoretic approach, mean-field approximation and computer simulations

Angelo Rosa
SISSA, Trieste, Italy

We introduce a novel, grand canonical field-theoretic formalism to study solutions of interacting polymer/solvent mixtures on the d -dimensional (hyper)cubic lattice. Albeit the theory does not admit an exact solution, its physical behavior can be conveniently understood by means of mean-field arguments that, as we show, (i) make the theory of the Flory-Huggins type and (ii) compare favorably well with Monte Carlo simulations [1]. Then, we extend the theory to a ternary mixture of polymer/solvent/vacancies [2] and show that it reproduces faithfully the properties of recent MD simulations for equivalent systems [3,4] and the molecular mechanism of polymer-assisted-condensation [5] advocated in the organization of chromatin inside the cells.

- [1]D. Marcato, A. Giacometti, A. Maritan, A. Rosa, *The Journal of Chemical Physics*, 159, (2023)
[2]D. Marcato, A. Giacometti, A. Maritan, A. Rosa, arXiv:2407.01590 (2024)
[3]Y. Huang, S. Cheng, *Journal of Polymer Science*, 59, 2819-2831 (2021)
[4]H. Garg, R. Rajesh, S. Vemparala, *The Journal of Chemical Physics*, 158, (2023)
[5]J. Sommer, H. Merlitz, H. Schiessel, *Macromolecules*, 55, 4841-4851 (2022)
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Tuesday 17/12/2024, 11:20 - 11:4

Surface and line adsorption in nanodroplets

Fabio Staniscia
Jožef Stefan Institute

We investigate, using molecular dynamics simulations, the behavior of nanodroplets made of solutions of surfactants in water, on hydrophilic and hydrophobic substrates. We characterize the adsorption properties at both water-vapor and water-substrate interfaces, and show that, for hydrophilic substrates, surfactant molecules can create an external film, adsorbed at the substrate-vapor interface, whose density depends on the substrate hydrophobicity. On top of adsorption at the interfaces, the system displays the presence of an excess of adsorbed surfactants close to the three-phase contact line. We characterize this phenomenon, showing that the contact line has a higher affinity for the adsorption than the interfaces.

Tuesday 17/12/2024, 11:40 - 12:00

Contact interactions in liquid-drop model

Fran Ivan Vrban, Antonio Šiber², and Primoz Ziherl^{1,3}

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2. Institute of Physics, Zagreb, Croatia
3. Jožef Stefan Institute, Ljubljana, Slovenia

Using the liquid-drop model [1] as an effective elasticity theory of microgels, we study contact interactions between such particles. We first numerically compute the equilibrium particle shapes characterized by faceting as well as the corresponding deformation energies, focusing on the simple cubic lattice. These results are then interpreted in terms of several model shapes described by one or two variational parameters. We find that generally, the so-called truncated spherocube shape performs best in both attractive and repulsive regime across a broad range of indentations and at any compressibility. Our work constitutes a basis of a coarse-grained description of mechanics of dense microgel suspensions.

[1] J. Riest, L. Athanasopoulou, S. Egorov, C. N. Likos, and P. Ziherl, *Sci. Rep.* **5**, 15854 (2015).

Tuesday 17/12/2024, 12:00 - 12:20

Active junctional fluctuation-driven ordering in 3D cellular aggregates

Tanmoy Sarkar
Jožef Stefan Institute

Order-disorder transitions in tissues are frequently observed during development and disease progression. However, the mechanics of such transitions in bulk three-dimensional (3D) tissues remain poorly understood. We investigate 3D cellular aggregates using the vertex model to address this gap. We employ active fluctuating tension at cellular junctions of these aggregates to explore their energy landscapes. Our results reveal that the cellular aggregates achieve efficient ordering at an intermediate amplitude of fluctuating tension. This ordered state is further supported by a non-monotonic response in the structure factor and pair correlation functions as the tension amplitude varies. Additional structural analyses, including edge length and shape factor distributions, indicate maximal order at intermediate amplitude levels. Furthermore, the dynamic behavior of the aggregates, characterized by the effective diffusivity of cells, reveals a transition from solid-like to fluid-like behavior, depending on the amplitude and persistence time of the fluctuating tension, particularly near the values where maximal order is observed.

Tuesday 17/12/2024, 12:20 - 12:40

Heterogeneous cavitation in water: Impact of surface defects and lipid coatings

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Liquids under tension are found in many systems in nature as well as in technology. Examples include lithotripsy and sonoporation of cell membranes [1,2], octopus suckers [3], catapulting

mechanisms of fern spores [4,5], and the hydraulic system in plants [6,7]. Such systems are metastable and vulnerable to cavitation. Aqueous systems containing lipid membranes and lipid-coated surfaces represent a cornerstone of biological systems. This raises a question: what role do lipids play in the process of cavitation? In this talk, I will present our work on the conditions that lead to catastrophic cavitation events in heterogeneous surface-water systems. We use a framework that combines classical nucleation theory with molecular dynamics simulations to model how the surface hydrophobicity, the presence of topographic defects, as well as the size of those defects affect the tensile strength of these systems. I will also discuss how lipids offer a stabilization mechanism against cavitation. We find that while pure bulk water is exceptionally stable against cavitation, the presence of even one nanoscopic surface defect is enough to destabilize water and reduce its tensile strength to experimentally measured values. Additionally, we find that a lipid coating increases the resistance against cavitation, especially for surfaces with defects.

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